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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyvinyl Alcohol and Poly Ethyl Urethane composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of poly vinyl alcohol and Poly ethyl Urethane to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of vinyl alcohol.This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Poly vinyl alcohol, Poly ethyl Urethane

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of

transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money.Thus, researchers have focused on the use of *In silico* approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.However, the polyvinyl alcohol (PVA) hydrogel is an intriguing hydrogel, which has been investigated as a promising substitute for repairing diseased or damaged articular cartilages, meniscuses and tendons due to its excellent biocompatibility, low toxicity and water absorption abilities [8-9]. Moreover, the researchers have used polyethylurethane polymers were chosen as drug carriers for α-tocopherol. This active ingredient is widely used as a strong antioxidant in many potential applications including medical and cosmetic, but is rapidly degraded, because of its light, heat and oxygen sensitivity [10]. This study is intended to identify the interaction of polyvinyl alcohol and polyethyl urethane to form blends.This study is intended to identify the interaction of poly vinyl alcohol and Poly ethyl urethane to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of poly vinyl alcohol_and Poly Ethyl Urethane were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of poly vinyl alcoholon the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of poly vinyl alcohol and Poly Ethyl Urethane as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties.For many years, group additive methods have been used to predict the properties of polymers and of small molecules. These methods are extremely fast and easy to use. Consequently, they are most useful when a rapid estimation of a property is needed without a thorough understanding of the atomic interactions that result in it. The key shortcoming of these approaches, however, is their dependency on a database of group contributions. Consequently, if a polymer includes a group for which the group contribution can not be determined, then that polymer 's property can not be measured.

To overcome this constraint, the method applied in Synthia uses topological polymer information in predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no group contribution database is needed and properties for any polymer composed of any combination of the following nine elements can be predicted: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine , bromine.

Bulk modulus: Bulk modulus is the measure of the decrease in volume with an increase in pressure. Figure 1 shows that the bulk modulus of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Shear modulus: It is defined as the ratio of shear stress and shear strain. It shows the response of the composite to shear deformation. Figure 2 shows that the shear modulus of the composite increases linearly with increase in mass fraction of vinyl alcohol

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Poisson ratio: It is the ratio of lateral strain to longitudinal strain. Figure 4 shows that the Poisson ratio of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Brittle fracture stress: Brittle Fracture is the sudden, rapid cracking of a material under stress where the material exhibited practically no evidence of ductility or plastic degradation before the fracture occurs.Figure 5 shows that the brittle fracture stress of the composite increases linearly with increase in mass fraction of vinyl alcohol.

CONCLUSION

The possibility of use of poly vinyl alcoholand Poly ethyl urethane to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to mechanical properties.The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of acrylic acid. Usually components for a blend are identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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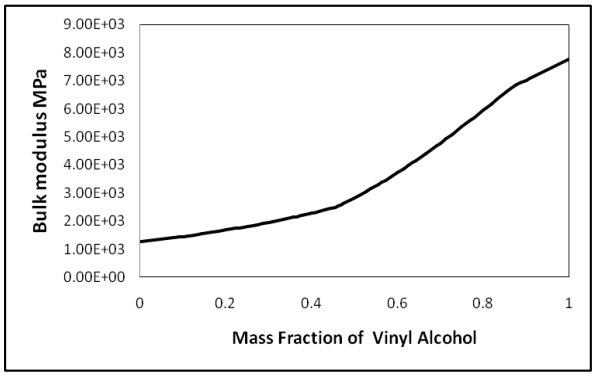

Figure 1. Change in bulk modulus with mass fraction of Vinyl Alcohol

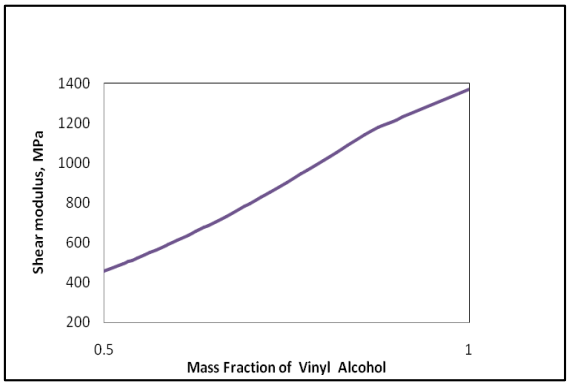

Figure 2. Change in shear modulus with mass fraction of Vinyl Alcohol

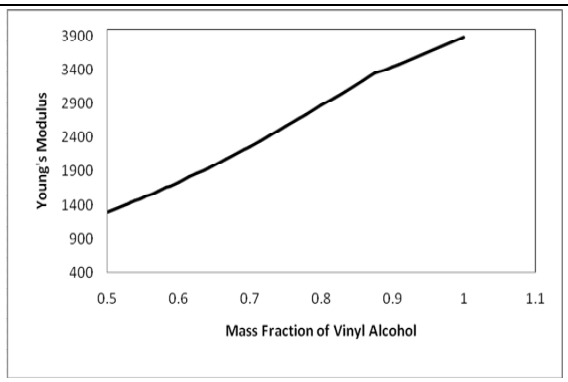

Figure 3. Change in Young's modulus with mass fraction of Vinyl Alcohol

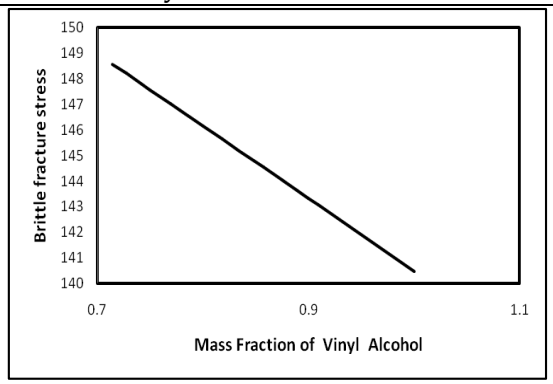

Figure 4. Change in Poisson modulus with mass fraction of vinyl alcohol

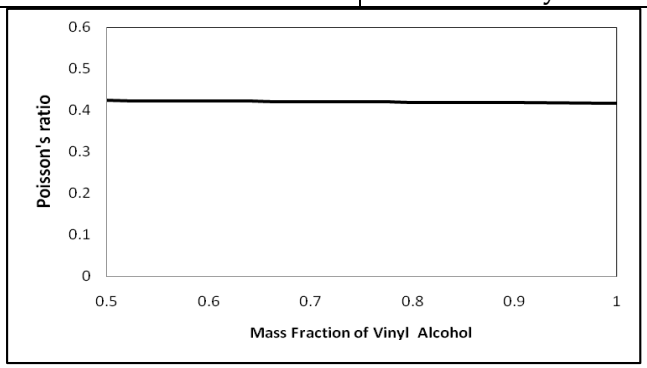

Figure 5. Change in brittle fracture stress with mass fraction of vinyl alcohol

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Keywords: Poly vinyl alcohol, Polyoxy ethylene

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Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

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Vinyl polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxilla facial appliances for skeletal defects etc. [8], bone repair [9], dispersing agent, super absorbent polymer, ion-exchange resin, etc.[10].Polyvinyl alcohol is a polyelectrolyte soluble in aqueous media at neutral pHIt is used for preparing hydrogels. It is not toxic and does not cause irritation [11]. Further, the polyvinyl alcohols (PVA) are a water soluble polymer and also susceptible of ultimate biodegradation in the presence of suitably acclimated microorganisms. Besides, this polymer blends possess good thermal stability [12]. Besides, Polyoxyethylene surfactants are widely used as emulsifying agents and detergents. This ionic surfactants form micelles above a critical concentration in water with liquid crystals frequently occurring at higher concentrations [12]. This study is intended to identify the interaction of polyvinyl alcohol and polyoxyethylene to form blends.

Researchers have used polyoxyethylene in combination with other materials to act as adsorbent [12]. polyoxyethylene have been reported to be used in Curtius reaction. This study is intended to identify the interaction of polyvinyl alcohol and polyoxyethylene to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

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To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties Asha Rani Dalai and Subhraraj Panda may be predicted for any

polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

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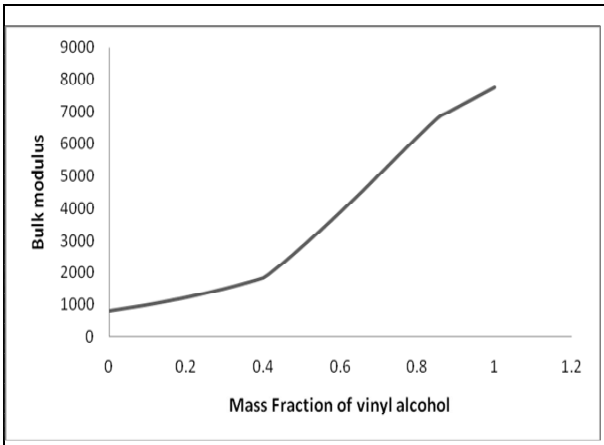

Figure 1. Change in bulk modulus with mass fraction of vinyl alcohol

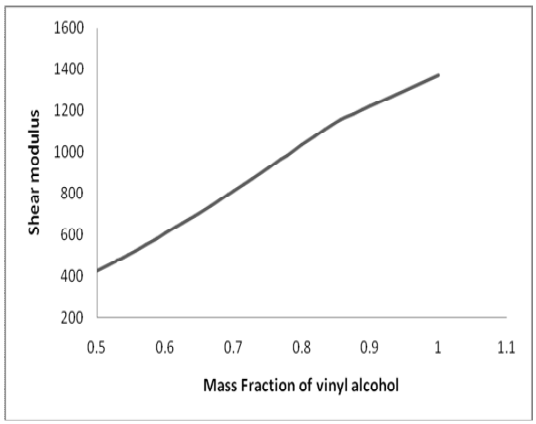

Figure 2. Change in shear modulus with mass fraction of Vinyl Alcohol

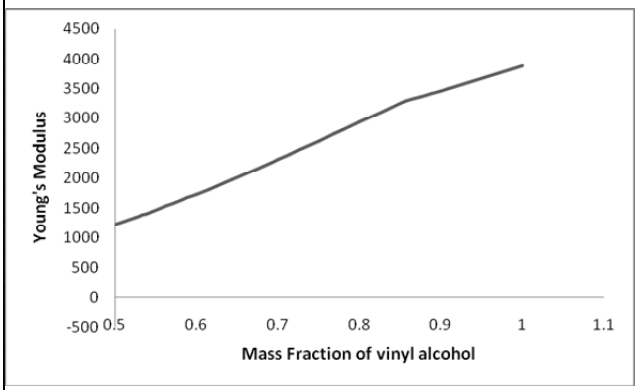

Figure 3. Change in Young's modulus with mass fraction of vinyl alcohol

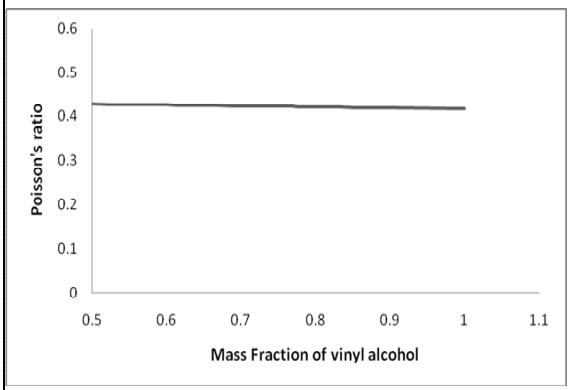

Figure 4. Change in Poisson modulus with mass fraction of vinyl alcohol

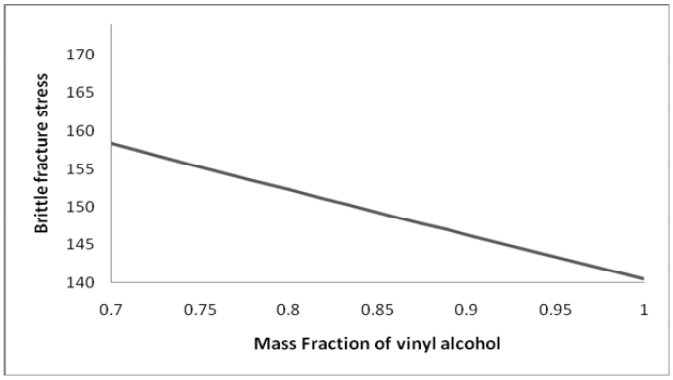

Figure 5. Change in brittle fracture stress with mass fraction of vinyl alcohol

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Polyacrylic acid is used as a electrolyte soluble in aqueous media at neutral pH, good adsorbent, hydrophobic, biocompatible and used as electrolyte [11]. Researchers have used polyacrylonitrile (PAN) is a carbon fiber precursor and is also used for activated carbon. However, the carbonized and activated electrospun PAN fibers are attractive for supercapacitor electrodes, catalysis, and other applications [12]. This study is intended to identify the interaction of polyacrylic acid and polyacrylonitrile to form blends.

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The possibility of use of acrylic acidand acrylonitrile to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to mechanical properties.The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of acrylic acid. Usually components for a blend are identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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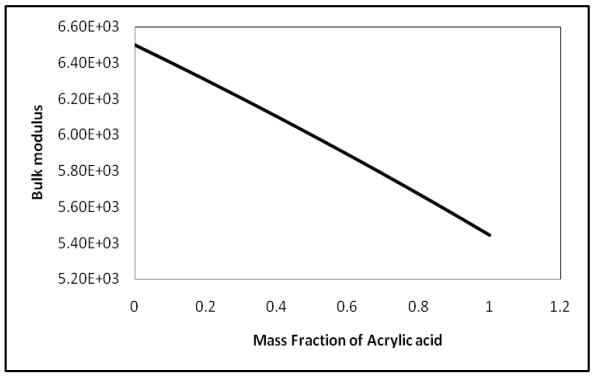

Figure 1. Change in bulk modulus with mass fraction of acrylic acid

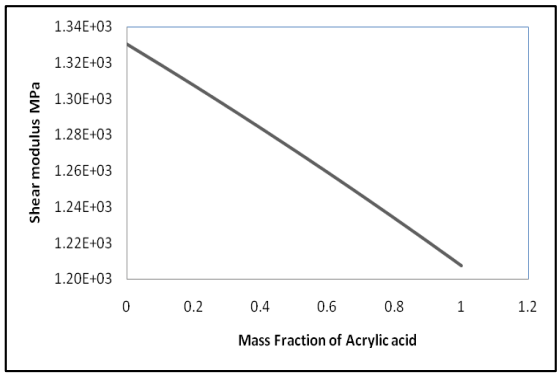

Figure 2. Change in shear modulus with mass fraction of acrylic acid

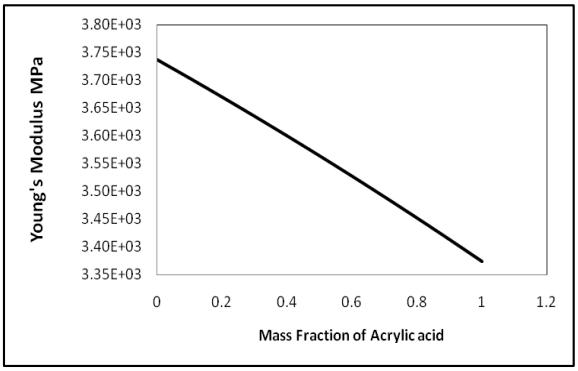

Figure 3. Change in Young's modulus with mass fraction of acrylic acid

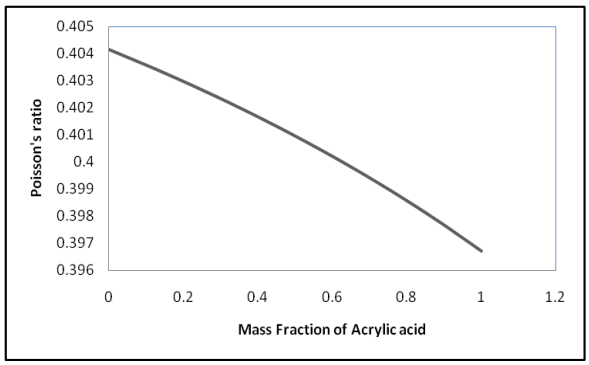

Figure 4. Change in Poisson modulus with mass fraction of acrylic acid

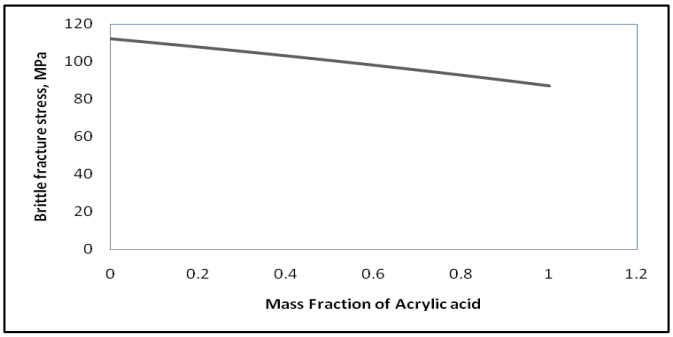

Figure 5. Change in brittle fracture stress with mass fraction of acrylic acid

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyvinyl Alcohol and Polyoxymethylene Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of poly Vinyl alcohol and polyoxy methylene to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of Vinyl alcohol.This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Poly vinyl alcohol, Polyoxy methylene composite

INTRODUCTION

Blends or composites are materials containing more than one components. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of

transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of *In silico* approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.vinyl polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denturerepair materials, maxillofacial appliances for skeletal defects etc. [8], bone repair [9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc.[10].Polyvinyl alcoholis a polyelectrolyte soluble in aqueous media at neutral pH. It is used for preparing hydrogels. It is not toxic and does not cause irritation [11]. Researchers have used polyoxymethylene in combination with other materials to act as adsorbent [12]. However, the physical properties of polyoxymethylene changes which occur during the rolling process of these polymers and these polymers possess good thermal and mechanical properties [13]. This study is intended to identify the interaction of polyvinyl alcohol and polyoxymethylene to form blends. This study is intended to identify the interaction of poly Vinyl alcohol and polyoxymethylene to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcoholand polyoxymethylene were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcoholand polyoxymethylene as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Bulk modulus: Bulk modulus is the measure of the decrease in volume with an increase in pressure. Figure 1 shows that the bulk modulus of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Shear modulus: It is defined as the ratio of shear stress and shear strain. It shows the response of the composite to shear deformation. Figure 2 shows that the shear modulus of the composite increases linearly with increase in mass fraction of Vinyl alcohol.

Young's modulus: It is defined as the ratio of stress and strain. It compares the relative stiffness of the composite. Figure 3 shows that the Young's modulus of the composite increases linearly with increase in mass fraction of Vinyl alcohol.

Poisson ratio: It is the ratio of lateral strain to longitudinal strain. Figure 4 shows that the Poisson ratio of the composite increases linearly with increase in mass fraction of Vinyl alcohol.

Brittle fracture stress: Brittle Fracture is the sudden, rapid cracking of a material under stress where the material exhibited practically no evidence of ductility or plastic degradation before the fracture occurs. Figure 5 shows that the brittle fracture stress of the composite increases linearly with increase in mass fraction of Vinyl alcohol.

CONCLUSION

The possibility of use of polyvinyl alcohol and polyoxymethylene to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to mechanical properties.The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of Vinyl alcohol. Usually components for a blend are identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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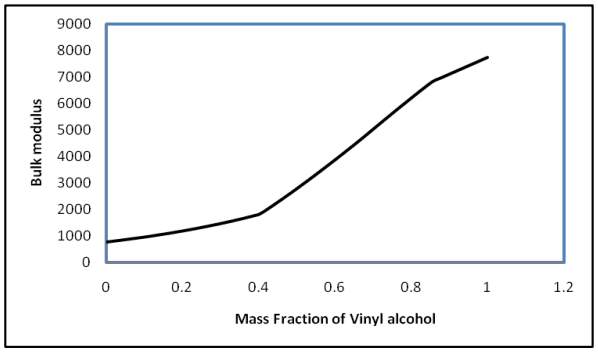

Figure 1. Change in bulk modulus with mass fraction of Vinyl alcohol

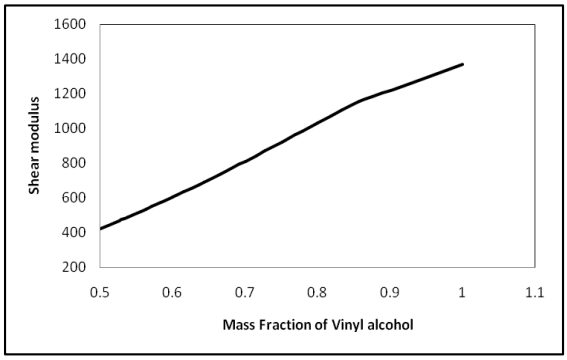

Figure 2. Change in shear modulus with mass fraction of Vinyl alcohol

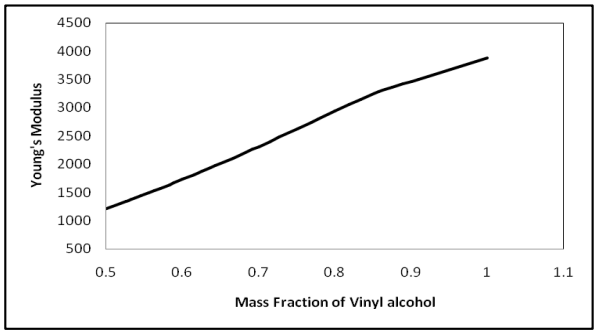

Figure 3. Change in Young's modulus with mass fraction of Vinyl alcohol

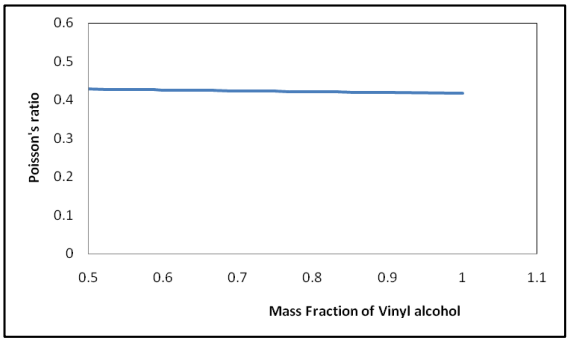

Figure 4. Change in Poisson ratio with mass fraction of Vinyl alcohol

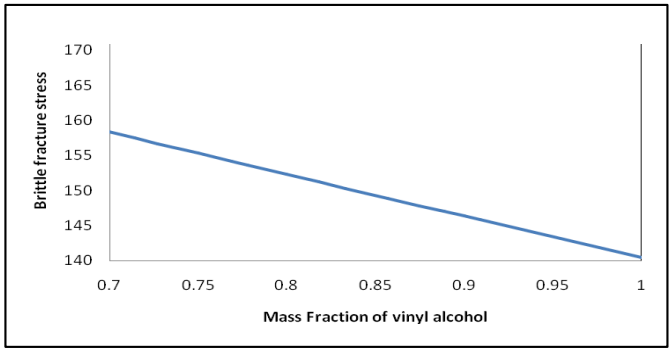

Figure 5. Change in brittle fracture stress with mass fraction of Vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyacrylic Acid and Polyacrylonitrile Composite

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Received: 16 Mar 2020 Revised: 18 Apr 2020 Accepted: 22 May 2020

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of polyacrylic acid and polyacrylonitrile to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in polyacrylic acid fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases decreased with increase in mass fraction of polyacrylic acid. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Poly acrylic acid, Polyacrylonitrile composite

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working

on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of *In silico* approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Among the various polymers, polyacrylic acid is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of polyacrylic acid is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, polyacrylic acid is non-toxic, good adsorbent, hydrophobic, biocompatible and used as electrolyte [11]. Researchers have used polyacrylonitrile (PAN) is a carbon fiber precursor and is also used for activated carbon. However, the carbonized and activated electrospun PAN fibers are attractive for supercapacitor electrodes, catalysis, and other applications [12]. This study is intended to identify the interaction of polyacrylic acid and polyacrylonitrile to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyacrylic acid and polyacrylonitrile were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyacrylic acid on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and polymer X as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated. To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine. To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of

group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite decreases linearly with increase in mass fraction of acrylic acid.

Density: Increase in density indicates decrease in porosity. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite decreases linearly with increase in mass fraction of acrylic acid.

Permeability of gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium.Lower permeability indicates longer time lag for the gas to pass through the mebrane. Figure 3 shows that the permeability of oxygenthrough the composite decreases with increase in mass fraction of acrylic acid.

Figure 4 shows that the permeability of nitrogenthrough the composite decreases with increase in mass fraction of acrylic acid. Figure 5 shows that the permeability of carbon dioxidethrough the composite decreases with increase in mass fraction of acrylic acid. Thus the results indicated that an increase in acrylic acid fraction reduces the permeability of different gases. The rate of permeability might be influence by the molecular weight of the gases.

CONCLUSION

The possibility of use of polyvinyl alcohol and polyethyl urethane to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in acrylic acid fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeability for all the gases decreased with increase in mass fraction of acrylic acid. Usually components for a blend are identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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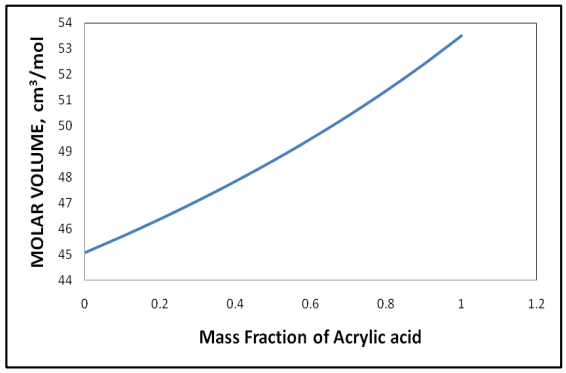

Figure 1. Change in molar volume with mass fraction of acrylic acid

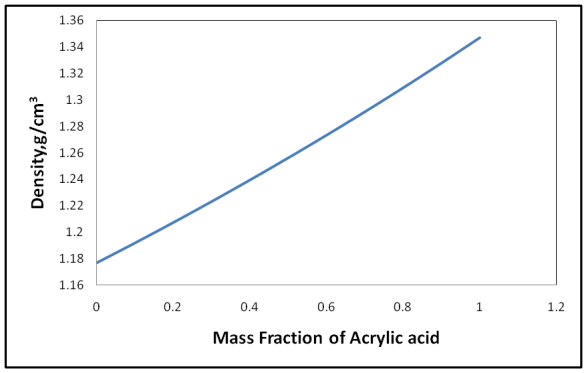

Figure 2. Change in density with mass fraction of acrylic acid

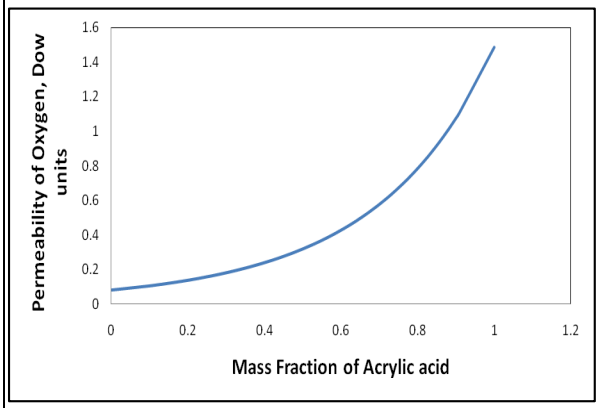

Figure 3. Change in permeability of oxygen with mass fraction of acrylic acid

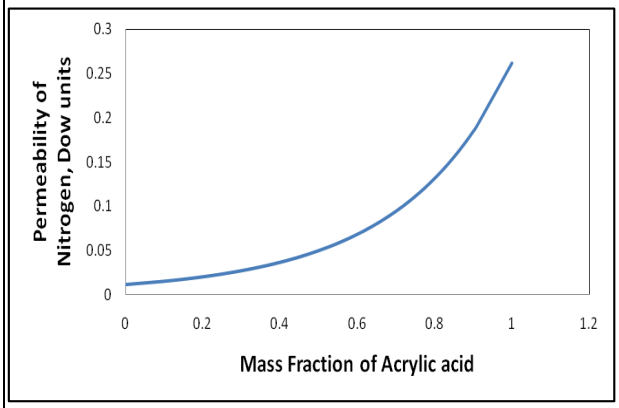

Figure 4. Change in permeability of nitrogen with mass fraction of acrylic acid

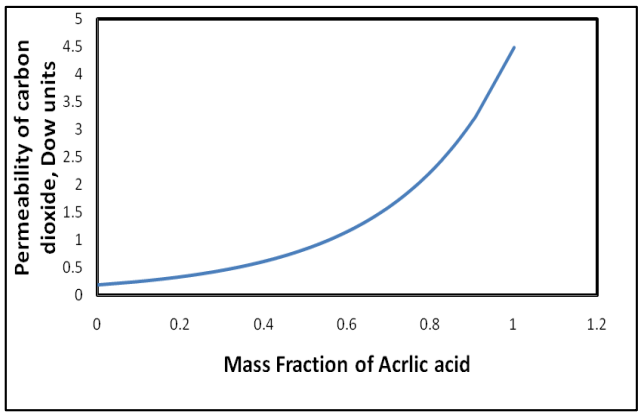

Figure 5. Change in permeability of carbon dioxide with mass fraction of acrylic acid

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RESEARCH ARTICLE

Investigation of Impedance and Modulus Study of Copper doped $SrTiO_3$

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ABSTRACT

The impedance and modulus study is performed at room temperature for different frequency ranges. The grain and grain boundary are responsible for conduction mechanism of $SrTiO_3$ by impedance spectroscopy. The dielectric and electrical properties of this material is strongly dependent on temperature and frequency. Jonscher's universal power law was followed by dependence of ac conductivity on frequency at different temperatures.

Keywords: Solid state reaction; Modulus; Impedance; AC conductivity;

INTRODUCTION

In recent years, Strontium titanate (STO) has gained a lot of attraction in the field of electronics because of itssignificant electro-chemical properties. It has high dielectric constant, high melting temperature, low coefficient of thermal expansion[1]. It is a ferroelectric perovskite material with face centered cubic structure[2]. Moreover, STO is an important band insulator because it has a band gap = 3.2 eV[3].It plays a vital role in photo-catalysts in solar cells, and solid oxide electronic devices[4]. It has been used in various microwave application because of its dielectric nonlinearity nature(dielectric constant depends on applied electric field) [5]. It has a vast application in the fields of RF filters, hydrocarbon sensors and antennas[6]. Doping of transition metals like Cu can enhance its ferroelectric properties. Cu oxide is a p-type semiconductor with 1.2 eV[7]. Cu doping can significantly affect its transport properties such as enhanced dielectric constant, low dielectric loss, improved ac conductivity, etc. [8]. There are several methods to synthesize STO but in this work, we have followed solid state methodto synthesize Cu doped STO ceramic powders and then made composite of these ceramic-polymers with the help of PMMA polymers by solution casting method and studied about how the Cu doping affects its electrical impedance and complex modulus which can give us an idea about the grain boundary, overall electrical properties, relaxation period, bulk properties and the various types of polarization occurring inside the material.

Experimental

The ceramic powders of Cu doped $SrTiO_3$ were prepared using high-temperature solid state reaction technique using high-purity stoichiometry ingredients. The structure weighed stoichiometrically was carefully blended, first for 2 hours in an air atmosphere and then for another 1 hour in alcohol. Then the mixed powders were calcinated at an optimized temperature of 950ºC for 4hr in a high purity alumina crucible. At first 0.025g of $(Pb_{0.5}Cu_{0.5})TiO_3$ was taken in a crucible and heated it for two hours with a temperature of 150ºC.Then the powder was grinded for 30 mins. Then 20ml of N, N-Dimethylformamide was taken in a conical flask and 5g of PMMA was added to it. The mixture is left at ambient temperature for 20 minutes under continuous magnetic stirring until a homogenous mixture is formed. Then to the above mixture stoichiometric (0.025g) amount of ceramic powder ($(Pb_{0.5}Cu_{0.5})TiO_3$) was added. Again, the mixture was stirred for 1hr and a homogeneous mixture was obtained. Then the homogeneous mixture was casted on glass Petridis and heated in a hot air oven at 120ºC for 4-5 hours. Finally, the polymer film was obtained.

RESULT AND DISCUSSION

Impedance Study

In order to analyze the transport properties of the material and nature of the material response, complex impedance analysis study is used [9] such as study the real and imaginary parts of some complex parameters impedance, modulus, etc. From the fig.1(a) we can analyze the variation of real part of impedance with frequency. It shows large value of impedance at lower frequency region but as soon as the frequency increases the impedance value falls suddenly and almost after 9 KHz onwards it attends saturation. Relatively low value saturation frequency indicates that heavier ion/dipole may be associated with some switching. This suggests the presence of mixed nature of polarization behavior in the material, such as electronic, dipolar and orientation polarization. These results indicate a possibility of increase in ac conductivity which is due to the release of space charge and lowering in the barrier properties of the material. Again, from graph 1(b), the variation of imaginary part of impedance with frequency can be studied. Here the value of Z"increases rapidly from the negative axis with increase in frequency and reaches a saturation at 20 KHz. This may happen due to presence of some voids.

Modulus Study

Fig.2(a) shows the variation of real part of modulus (M') with frequency which shows a dispersion tending towards M′ (the asymptotic value of M' at higher frequencies) and the dispersion shifts towards higher frequency sideas the frequency increases. The asymmetric plot of M' is because of the stretched exponential character of relaxation time of the material. The monotonous dispersion on increasing frequencymay be because of short range mobility of charge carriers. This is may be due to lack of restoring force governing the mobility of the charge carriers under the action of an induced electric field [10]. On the other hand, the variation of imaginary part of modulus (M") can be explained by fig.2(b). From this graph it can be seen that at higher frequency range M" shows a strong peak at 2000KHz. The frequency region below peak maximum M" determines the range in which charge carriers are mobile on long distances. At frequency above peak maximum, the carriers are confined to potential wells, being mobile on short distances.

Conductivity Study

Fig.3 explains the variation of ac conductivity with frequency. It increases with increase in frequency and between reaches a maximum value of 4.934 ohm-1m-1 at a frequency of 4000kHz. At low frequency the charge accumulation at the electrode-interface takes place which reduces the conductivity. The high frequency region of the ac conductivity is frequency independent due to the random diffusion of the ionic charge carriers and the values correspond to dc conductivity.

CONCLUSION

The ferroelectric composites of Cu doped $SrTiO_3$ are successfully prepared by high-temperature solid state technique. The doping of Cu enhances the conductivity of the composite. These studies reveal a significant contribution of grain and grain boundary effect in the material. The frequency dependent real impedance shows that at low temperature region space charge polarization is released.

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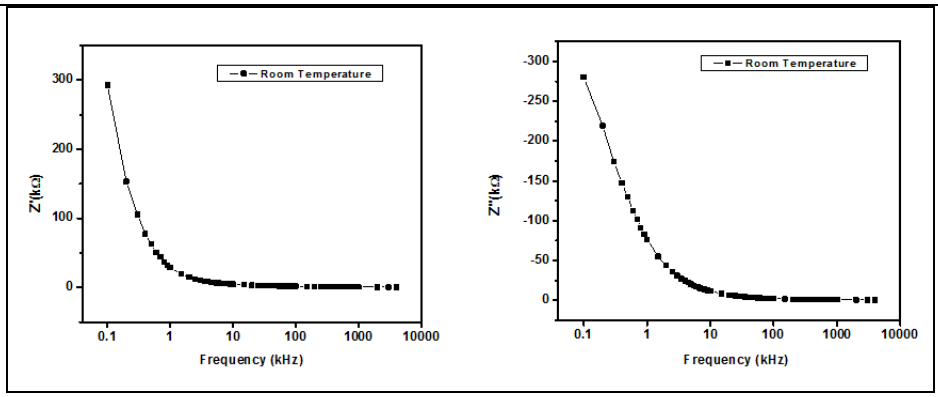

Fig 1 (a) and (b):variation of real and imaginary impedance as a function of Frequency (kHz)at room temperature Cu doped $SrTiO_3$

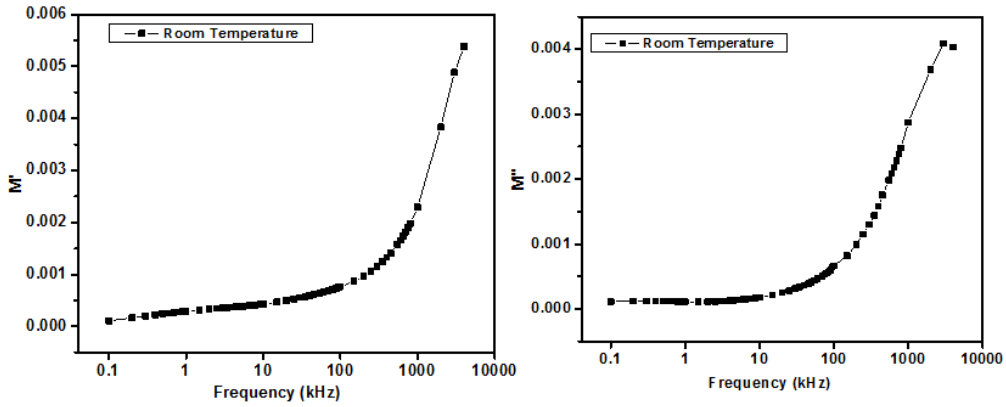

Fig 2 (a) and (b):variation of real and imaginary modulus as a function of Frequency (kHz)at room temperature Cu doped $SrTiO_3$

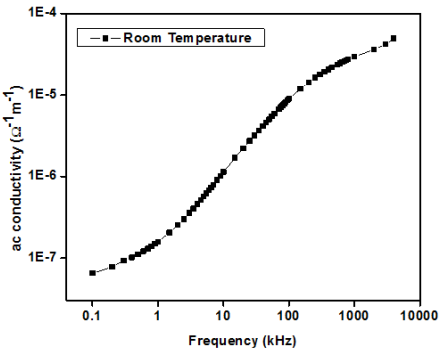

Fig 3: variation of conductivity as a function of Frequency (kHz)at room temperature Cu doped $SrTiO_3$

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RESEARCH ARTICLE

In silico Analysis of Polyvinyl Alcohol and Polyoxy Ethylene Compatibility in a Blend

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ABSTRACT

A blend is formed with the combination of two or more components. The compatibility of polyvinyl alcohol and polyoxy ethylene were studied to form a miscible blend with the tool, Biovia Materials Studio. The compatibility of the two components was verified with free energy of mixing, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible only at high temperature. Phase diagram indicated that a single phase can be obtained above 700 K which was the critical temperature. The coordination number was found to be 5.69 +/- 0.04. The highest number of configurations with respect to energy level was found to be -1.95kcal/mol. This study will not only help to determine pairs without performing laboratory experiments but also less time consuming and low cost process.

Keywords: Blend, *In silico*, polyvinyl alcohol, polyoxy ethylene.

INTRODUCTION

Blends or composites are formed with combination of more than one component where components do retain their identity in the mixture. Since it is very rare to find multiple properties in a pure material, so one can combine different components for improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi-functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering owing to its high value of strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method andthis technique is a low cost and less time consuming method. Thus, researchers have focused on the use of *In silico* approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs. Polyvinyl alcohol (PVA) isone of the most interesting material owing to its high value of dielectric strength, adhesiveness,easy film formation and also its properties can be improved by various dopant concentrations [8, 9]. Strong polymeric films are produced for the packaging industry since PVA film is easy to fabricate.This is owing to their high mechanical strength, highly stable and can be easily processed [10]. In addition, PVA is non-toxic, hydrophilic, semi crystalline, biocompatible and easily soluble in water [11].Researchers have found applications of polyvinyl alcohol (PVA) are a water soluble polymer and also aresusceptible for biodegradation, in the presence of acclimated microorganisms. Besides, this polymer blends possess good thermal stability [12]. On the other hand, Polyoxyethylene surfactants are popularly used as emulsifying agents and detergents. Above a critical concentration, this ionic surfactants form micelles in water, with liquid crystals forming at higher concentrations [13]. This study is intended to identify the interaction of polyvinyl alcohol and polyoxyethylene to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software package (Dassault Systemes of France) was used for this work and its analysis. The software uses machine learning techniques and standard algorithms to predict the results.

Methodology: Polyvinyl alcohol and polyoxyethylenewere prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyvinyl alcohol was used as the base and polyoxyethylenewas used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and polyoxyethylene as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy: A blend is known as amiscible if it is homogeneous. If the free energy has a negative value that indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$\Delta G_m = \Delta H_m \quad T\Delta S_m$ (1)

where ΔG_m = Gibbs free energy of mixing

ΔH_m = Enthalpy of mixing

ΔS_m = Entropy of mixing

T = Absolute temperature

The value of $T\Delta S_m$ is always positive in case of a blend as the entropy increases after the mixing. Thus, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components gets added to form a miscible blend only when the contribution of entropy to free energy is more than the contribution from enthalpy, i.e.,

$\Delta H_m < T\Delta S_m$ (2)

Figure 1 shows that the free energy involved in mixing is always negative or less than zero for the temperatures studied. The free energy is inversely proportional to temperature (upto 275 K) as evident from Eq. 1 and then free energy increases with increase in temperature. The results indicated that the blend will not lead to a homogeneous mixture for the temperature range studied (50 to 500 K). The trend shows a very good compatibility between polyvinyl alcohol and poly polyoxyethylene with negative value of mixing energy, which may lead to form a perfect blend with significantly less effort.

Chi Parameter: The free energy of mixing is described by the Flory–Huggins χ parameter and helps to explain phase behavior for polymer blends and block copolymers. The polymers which are not chemically similar, a significant difference in cohesive energy density leads to a high χ value and that indicates a larger driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicates poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture to occupy the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in stiffness of the chain for chemically similar components may lead to a high positive value of χ (chi).

Figure 2 shows that the χ value is high for the temperature range studied (50 to 500 K) indicating de-mixing. The χ value decreased with increase in temperature.Thus at high temperature there is a possibility to form a miscible blend.This agrees with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated considering all possible molecular pairs those are involved in the molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used off-lattice calculations. It is assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only in case of the components of the binary blend having similar volumes or similar surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are of different sizes. In this study the coordination number was found to be 6.97 +/- 0.04.

Phase Diagram: The phase diagram is used to understand the compatibility of binary mixtures. Figure 3 shows the phase diagram for the two components of the blend. There are three regions with different degree of miscibility:

a. The single-phase miscible region existed above the critical temperature of around 750 K. This value supported the fact that a single phase blend can be formed at a high temperature (higher than 750 K).

b. Fragmented metastable region existed inbetween binodals region and spinodals region, and

c. The two-phase separated regions of immiscibility are bordered by the spinodals.

The binodals separated miscible (one-phase) and metastable region, while the spinodals separated the met stable and two-phase region.

When the system moves from single-phase to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e., slow nucleation followed by growth of the phase separated domains. On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 5 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -1.95kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 6 shows that the mixing energy for the system was small for the temperature range studied. The graph indicated that an increase in temperature increased the mixing energy. It also shows that mixing energy gradually increases with increase intemperature with varying the temperature from 50 K to 500 K. So, it is very much possible to mix the two components at any feasible temperature with least mixing energy value. The formation of non homogeneous blend with polyvinyl alcohol as base might help formation of blend with high mechanical strength. This might have an application as packaging material and adsorbent.

CONCLUSION

The possibility of use of polyvinyl alcohol and polyoxy ethylene to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair can have very good compatibility at different ranges of temperature. The coordination number was found to be 5.69 +/- 0.04. The maximum number of configurations with respect to energy level was found to be -1.95kcal/mol. usually components for a blend are identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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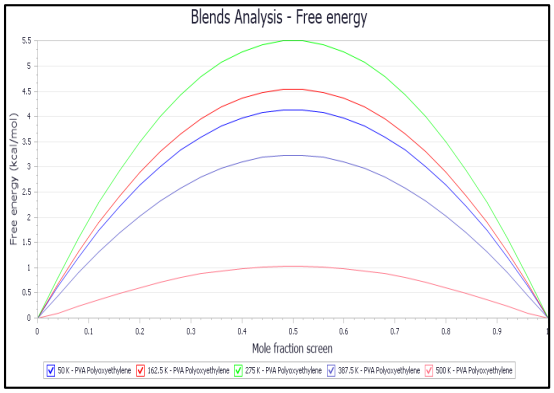

Figure 1. Free energy change with mole fraction of polyoxyethylene at different temperatures

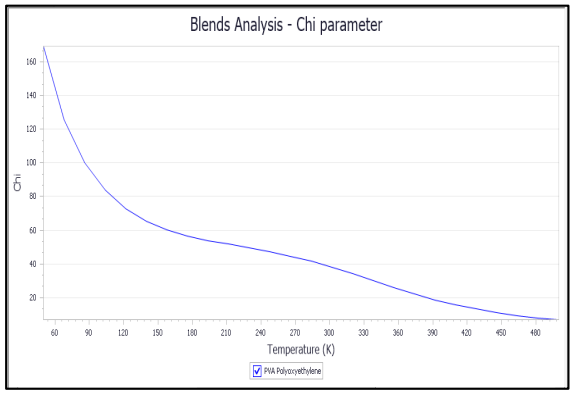

Figure 2. Change in χ (chi) value with temperature

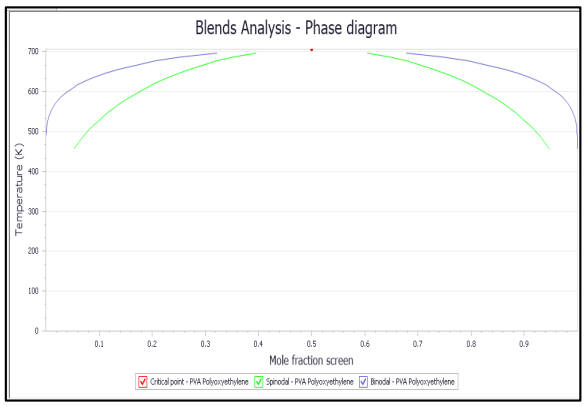

Figure 3. Phase diagram

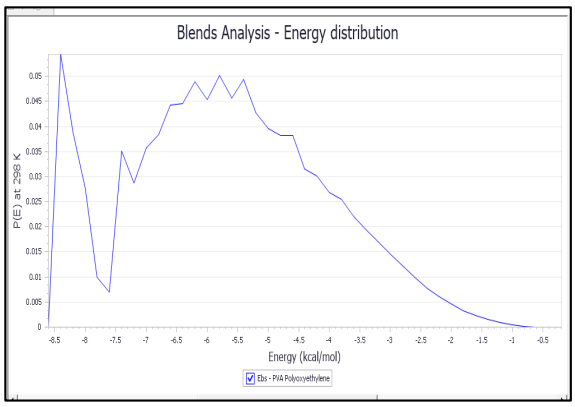

Figure 4. Energy distribution

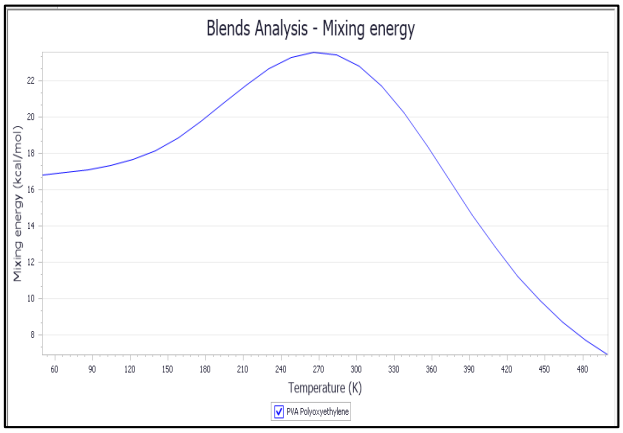

Figure 5. Mixing energy

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RESEARCH ARTICLE

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Keywords: Blend, *In silico*, polyvinyl alcohol, polyoxymethylene

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Blends or composites are formed with combination of more than one component where components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisableto combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working

on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high value of strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method andthis technique is a low cost and less time consuming method. Thus, researchers have focused on the use of *In silico* approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs. Polyvinyl alcohol (PVA) isone of the most interesting material owing to its high value of dielectric strength, adhesiveness, easy film formation and also its properties can be improved by various doping of different concentrations [8, 9]. Strong polymeric films are produced for the packaging industry since PVA film is easy to fabricate.This is owing to their high mechanical strength, highly stable and can be easily processed [10]. In addition, PVA is non-toxic, hydrophilic, semi crystalline,biocompatible and easily soluble in water [11]. Researchers have found the most dominating property of polyvinyl alcohol is thermal resistance [12]. However, the physical properties of polyoxymethylene changes which occur during the rolling process of these polymers and these polymers possess good thermal and mechanical properties [13]. This study is intended to identify the interaction of polyvinyl alcohol and polyoxymethylene to form blends.

MATERIALS AND METHODS

Software Used: For this work the Biovia software tool has been used. Its a software tool developed by DassaultSystemesof France. All analysis were done by Materials studio that is a module of Biovia software. The software uses machine learning techniques and standard algorithms to predict the results.

Methodology: Polyvinyl alcohol and polyoxymethylene were prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyvinyl alcohol was used as the base and polyoxymethylene was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol andpolyoxymethylene as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy: A blend is known as amiscible if it is homogeneous. If the free energy has a negative value that indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where ΔG_m = Gibb's free energy of mixing

ΔH_m = Enthalpy of mixing

ΔS_m = Entropy of mixing

T = Absolute temperature

The value of $T\Delta S_m$is always positive in case of a blend as the entropy increases for mixing. Thus, the sign of $\Delta G_m$is found to depend on the value of the enthalpy of the mixing ΔH_m. The components gets added to creat a miscible blend only when the contribution of entropy to free energy is more than the contribution from enthalpy, i.e.,

$\Delta H_m < T\Delta S_m$ (2)

Figure 1 shows that the free energy involved in mixing is always negative or less than zero for the temperatures studied. The free energy is inversely proportional to temperature (upto 275 K) as evident from Eq. 1 and free energy increases with increase in temperature. The results indicated that the blend will not lead to a homogeneous mixture for the temperature range studied (50 to 500 K). The trend shows a very good compatibility between polyvinyl alcoholand poly polyoxymethylene with negative value of mixing energy, which may lead to form a perfect blend with significantly less effort.

Chi Parameter: The free energy of mixing is described by the Flory–Huggins χ parameter and helps to explain phase behavior for polymer blends and block copolymers. Thepolymers which are not chemically similar, a significant difference in cohesive energy density leads to a high χ value and that indicates a larger driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicates poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture to occupy the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similar components may lead to a high positive value of χ (chi).

Figure 2 shows that the χ value is high for the temperature range studied (50 to 500 K) indicating demixing. The χ value decreased with increase in temperature.Thus at high temperature there is a possibility to form a miscible blend.This agrees with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated considering all possible molecular pairs those are involved in the molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used off-lattice calculations. It is assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only in case of the components of the binary blend having similar volumes or similar surface areas. It is difficult to apply the pairs method to define the coordination number for a binary system in which the components are not comparable in size. In this study the coordination number was found to be 4.97 +/- 0.04.

Phase Diagram: The phase diagram is used to understand the compatibility of binary mixtures. Figure 3 shows the phase diagram for the two components of the blend. There are three regions of different degree of miscibility:
a. The single-phase miscible region existed above the critical temperature of around 750 K. This value supported the fact that a single phase blend can be formed at a high temperature (higher than 750 K).
b. Fragmented metastable region existed in between binodals region and spinodals region, and
c. The two-phase separated regions of immiscibility are bordered by the spinodals.

The binodals separated miscible (one-phase) and metastable region, while the spinodals separated the metastable and two-phase region. When the system enters from single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e, slow nucleation followed by growth of the phase separated domains. On the other hand, when the system jumps from a single-phase to the spinodal region of immiscibility the phases separate automatically by a methodknown as spinodal decomposition.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 5 shows the plot of frequency (P(E)) against energy levels. It shows

that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -2.00 kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 6 shows that the mixing energy for the system was small for the temperature range studied. The graph indicated that an increase in temperature increased the mixing energy. It also shows that mixing energy gradually increases with increase intemperature with varying the temperature from 50 K to 500 K. So, it is very much possible to mix the two components at any feasible temperature with least mixing energy value. The formation of nonhomogeneous blend with polyvinyl alcohol as base might help formation of blend with high mechanical strength. This might have an application as packaging material and adsorbent.

CONCLUSION

The possibility of use of polyvinyl alcoholand polyoxymethylene to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair can have very good compatibility at different ranges of temperature. The coordination number was found to be 4.97 +/- 0.04. The maximum number of configurations with respect to energy level was found to be -2.3 kcal/mol. Usually components for a blend are identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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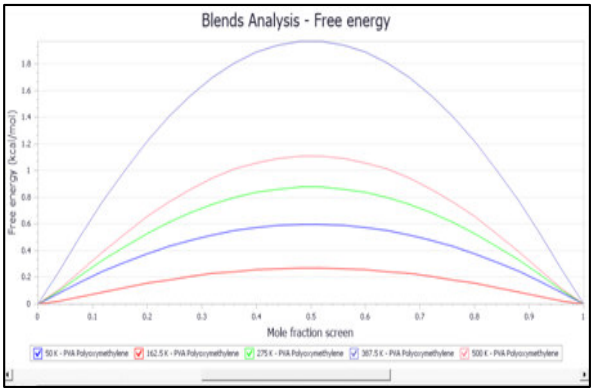

Figure 1. Free energy change with mole fraction of polyoxymethylene at different temperatures

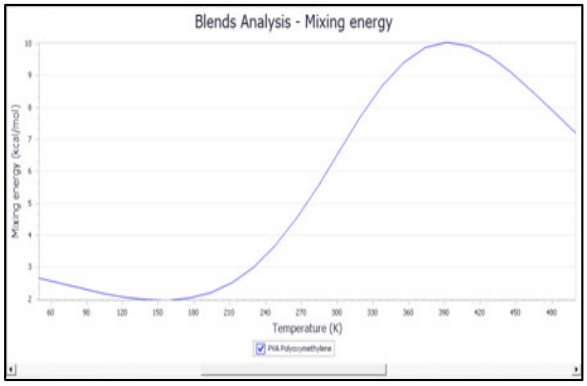

Figure 2. Change in χ (chi) value with temperature

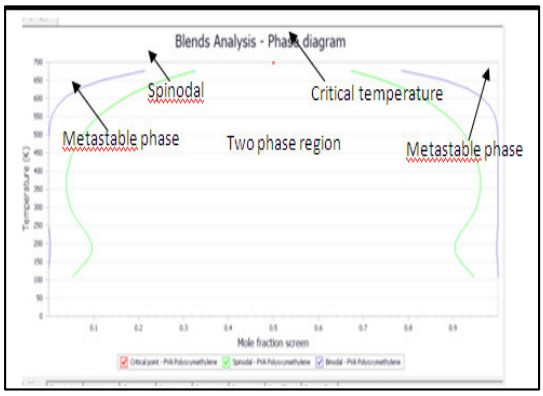

Figure 3. Phase diagram

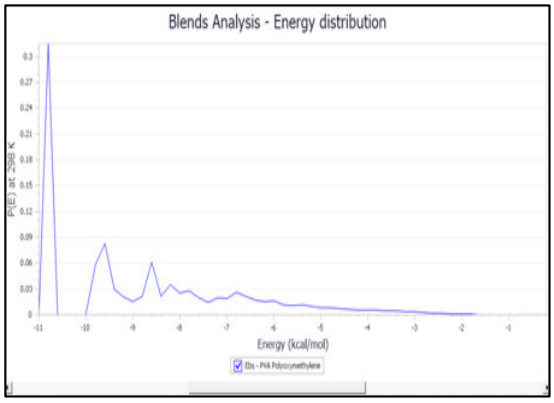

Figure 4. Energy distribution

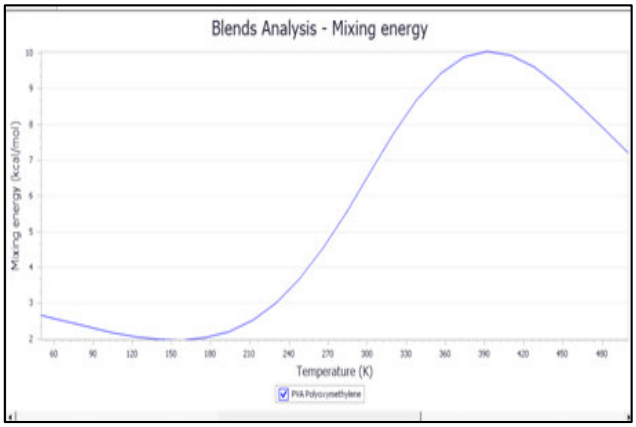

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyvinyl Alcohol and Urea Composite

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ABSTRACT

A blend is a mixture of more than one components. The desired property of a blend is its homogeneity. The composition of polyvinylalcohol and urea to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in polyvinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases decreased with increase in mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Blend, *In silico*, polyvinyl alcohol, Urea composite

INTRODUCTION

Blends or composites are materials containing more than one components. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of

lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering owing to its high value of strength to weight ratio and resistance to corrosion.Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money.Thus, researchers have focused on the use of *In silico* approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Polyvinyl alcohol (PVA) isone of the most interesting material owing to its high value of dielectric strength, adhesiveness, easy film formation and also its properties can be improved by various dopant concentrations [8, 9]. Strong polymeric films are produced for the packaging industry since PVA film is easy to fabricate.This is owing to their high mechanical strength, highly stable and can be easily processed [10]. In addition, PVA is non-toxic, hydrophilic, semi crystalline, biocompatible and easily soluble in water [11]. Researchers have used polyvinyl alcohol in combination with other materials to act as adsorbent [12].Also, the elastomeric thermoset polyurea has severallatest applications,like, increasing the life of structures under heavy loading and withstanding the case of blast and ballistic events [13]. This study is intended to identify the interaction of polyvinyl alcohol and urea to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software package (Dassault Systemes of France) was used for this work and its analysis. The software uses machine learning techniques and standard algorithms to predict the results.

Methodology: The structures of polyvinyl alcohol and urea were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and urea as potential components of a composite was analyzed using Materials Studio of Biovia. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a various polymer properties.Since long, group additive methods were used to study the properties of polymers and also that of small molecules. These methods are very fast and can be handled with ease.That is why they are popular especially forquick estimation of properties without going to the details of the intermolecular interactions which is actually the basic cause of it. However, the main drawback of these methods is their dependence upon a database of group contributions. Thus, in case of a polymer that contains a group, for which the group contribution cannot be predicted, then the properties of that polymer cannot be estimated.

To overcome this limitation, the method used in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices obtained from graph theory are used here. Thus, no database of group contributions is required and the properties can be estimated for any polymer consisting of any combination of the elements: C, H, N, O, Si, S, F, Cl and Br.

Molar volume: The volume occupied by one mole of a substance is called its molar volume. Figure 1 shows that the molar volume of the composite decreases linearly with increase in mass fraction of polyvinyl alcohol

Density: Increase in density indicates decrease in porosity. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Permeability of gas: under equilibrium condition, we can deifne Permeability as the rate at which the gas can pass through the polymer membrane. Lower permeability indicates longer time lag for the gas to pass through the mebrane. Figure 3 shows that the permeability of oxygenthrough the composite decreases with increase in mass fraction of Vinyl alcohol

Figure 4 shows that the permeability of nitrogenthrough the composite decreases with increase in mass fraction of Vinyl alcohol. Figure 5 shows that the permeability of carbon dioxidethrough the composite decreases with increase in mass fraction of Vinyl alcohol. Thus the results indicated that an increase in Vinyl alcohol fraction reduces the permeability of different gases. The rate of permeability might be influence by the molecular weight of the gases.

CONCLUSION

The possibility of use of polyvinyl alcohol and polyurea to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties.The molar volume and density decreased with increase in polyvinyl alcoholfraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeabilityfor all the gases decreased with increase in mass fraction of polyvinyl alcoholusually components for a blend are identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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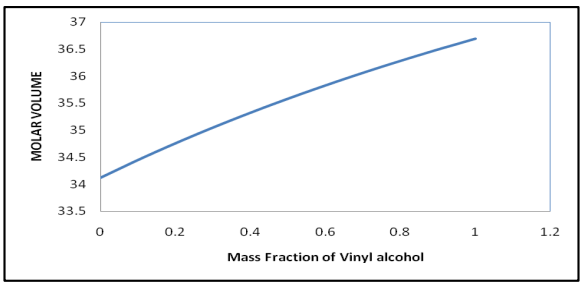

Figure 1. Change in molar volume with mass fraction of polyvinyl alcohol

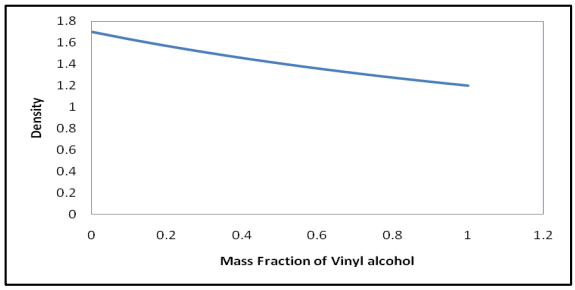

Figure 2. Change in density with mass fraction of vinyl alcohol

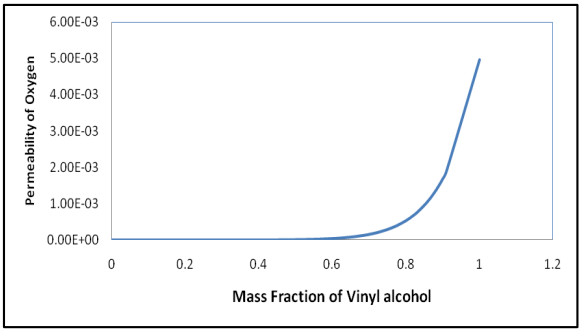

Figure 3. Change in permeability of oxygen with mass fraction of Vinyl alcohol

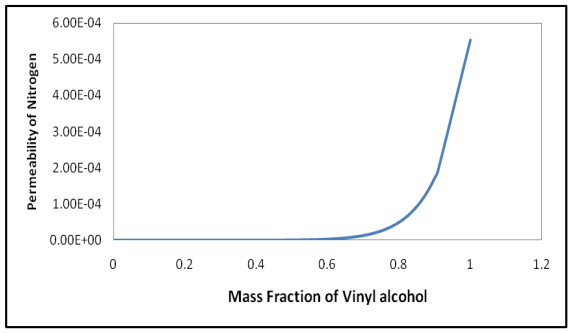

Figure 4. Change in permeability of nitrogen with mass fraction of Vinyl alcohol

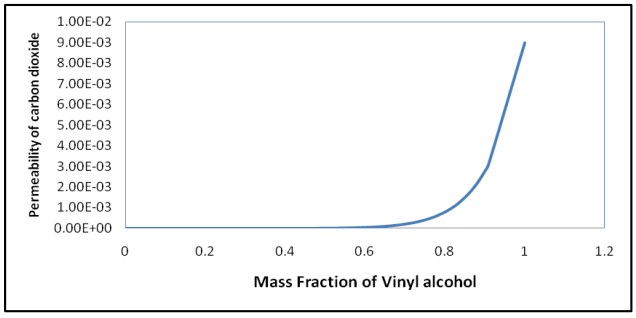

Figure 5. Change in permeability of carbon dioxide with mass fraction of Vinyl alcohol

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RESEARCH ARTICLE

Synthesis and Characterization of Copper Doped Perovskite Materials

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ABSTRACT

Ceramic powders of Cu doped Lead titanate ($Pb_{0.5}Cu_{0.5}TiO_3$) are synthesized through high temperature solid state reaction method. 5% of ceramic filler in to the polymer matrix was prepared by solution casting techniques. The Impedance studies of this polymeric composite were characterized by LCR meter in the wide range of frequencies from 10^2-10^6 Hz at room temperature. Moreover, Modulus study of the material can be done between the frequency ranges 10^2-10^6 Hz. Moreover, the Jonscher's universal power law was followed by dependence of ac conductivity on frequency at different temperatures.

Keywords: Solid state reaction; Modulus; Impedance; AC conductivity;

INTRODUCTION

In recent decades, materials scientists are showing much more interest in the development of new multifunctional ceramic, polymer, polymeric composite for various applications in the fields of electronics and optoelectronics. Keeping an eye on the above demands, polymeric crystals, especially ferroelectric polymer-ceramic composites has gained a huge attention due to their significant role in the devices like thin film capacitors, electronic transducers, pyroelectric sensors and nonlinear optics etc [1].

A composite is a mixture of two or more different materials of different phases having different properties which produce the desired material which may not be achieved in single-phase materials [2]. Ferroelectric polymer ceramics have been in demand because of their significant properties which make them ideal for photovoltaic process which is core concept of the energy storage devices [3]. The electrical energy density can be expressed by the formula $U = (\varepsilon r Eb^2)/2$ where εr is the dielectric constant of the material and Eb is the breakdown strength. To increase the electrical energy storage capacity, both high value of dielectric constant and large coefficient of breakdown strength are needed. Ceramic materials have high dielectric constant but their stiff and brittle nature make them lack in breakdown strength. On the other hand, polymers have low dielectric constant but large breakdown strength which makes them flexible so if the large dielectric constant of ceramics and high breakdown strength can be combined together then a suitable material for the energy storage application will be obtained [4].

Experimental Technique

The ceramic powder of Cu doped $PbTiO_3$ was prepared using high-temperature solid state reaction technique using high-purity stoichiometry ingredients. The structure weighed stoichiometrically was carefully blended, first for 2 hours in an air atmosphere and then for another 1 hour in alcohol. Then the mixed powders were calcinated at an optimized temperature of 950°C for 4hr in a high purity alumina crucible. Initially, 0.025g of $(Pb_{0.5}Cu_{0.5})$ TiO_3 was taken in a crucible and heated it for two hours with a temperature of 150°C.Then the powder was grinded for 30 mins. Then 20ml of N, N-dimethylformamide was taken in a conical flask and 0.5g of PMMA was added to it. The mixture is left at ambient temperature for 20 minutes under continuous magnetic stirring until a homogenous mixture is formed. Then to the above mixture stoichiometric (0.025g) amount of ceramic powder $[Pb_{0.5}Cu_{0.5})TiO_3]$ was added. Thus, the mixture was stirred for 1hr and a homogeneous mixture was obtained. Then the homogeneous mixture was casted on glass Petridis and heated in a hot air oven at 120°C for 4-5 hours. Finally, the polymer film was obtained. For electrical measurements, the polymer film faces were coated with high purity silver paste and dried at 100°C. The formation and structural properties of the compounds were studied by X-Ray diffraction (Rigaku, Ultima IV). Dielectric and impedance measurements were performed using an LCR meter computed (Impedance analyzer, IM 3570).

RESULTS AND DISCUSSION

Impedance and Modulus Study

In order to analyze the transport properties of the material and nature of the material response, complex impedance analysis study is used [7] such as study the real and imaginary parts of some complex parameters impedance, modulus, etc., Fig.1 shows the variation of real part of impedance with frequency. It is observed that the large value of impedance at lower frequency region but as the frequency increases the impedance value falls suddenly and almost after 9 KHz onwards it attends saturation. Relatively low value saturation frequencyindicates that heavier ion/dipole may be associated with some switching. This suggests the presence of mixed nature of polarization behavior in the material, such as electronic, dipolar and orientation polarization. These results indicate a possibility of increase in ac conductivity, which is due to the release of space charge and lowering in the barrier properties of the material.

As shown in Fig.2, the variation of imaginary part of impedance with frequency can be studied. Here the value of Z"increases rapidly from the negative axis with increase in frequency and reaches a saturation at 20 KHz. This may happen due to presence of some voids. Fig.3 shows the variation of real part of modulus (M') with frequency which shows a dispersion tending towards M' (the asymptotic value of M' at higher frequencies) and the dispersion shifts towards higher frequency side as the frequency increases. The asymmetric plot of M' is because of the stretched exponential character of relaxation time of the material. The monotonous dispersion on increasing frequency may be because of short range mobility of charge carriers.This is may be due to lack of restoring force governing the mobility of the charge carriers under the action of an induced electric field [8]. On the other hand, the variation of imaginary part of modulus (M'') can be explained by Fig.4. As shown in Fig.4, it can be seen that at higher frequency range M'' shows a strong peak at 2000 KHz. The frequency region below peak maximum M'' determines the range in which charge carriers are mobile on long distances. At frequency above peak maximum, the carriers are confined to potential wells, being mobile on short distances.

Conductivity Study

Fig.5 shows the variation of ac electrical conductivity with frequency at room temperature. It is observed that the increases with increase in frequency and in between 2000 KHz to 3000 KHz range it nearly saturates and beyond this range, it again increases and reaches to a value of 1.3919 $ohm^{-1}m^{-1}$ at 4000 kHz. At low frequency the charge accumulation at the electrode-interface takes place which reduces the conductivity. The high frequency region of the ac conductivity is frequency independent due to the random diffusion of the ionic charge carriers and the values correspond to dc conductivity.

CONCLUSION

The ferroelectric composites of Cu doped $PbTiO_3$ are successfully prepared by high-temperature solid state technique. The doping of Cu enhances the conductivity of the composite. These studies reveal a significant contribution of grain and grain boundary effect in the material. The results demonstrate that the composites effectively improve the dielectric performance and thus providing an excellent candidate for the development of energy storage devices.

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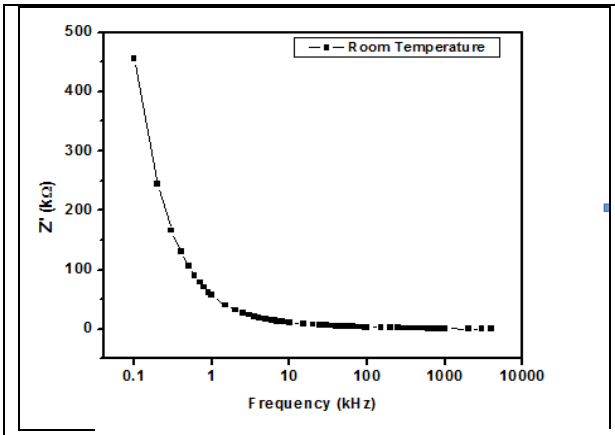

Fig.1: Variation of real part of impedance with frequency

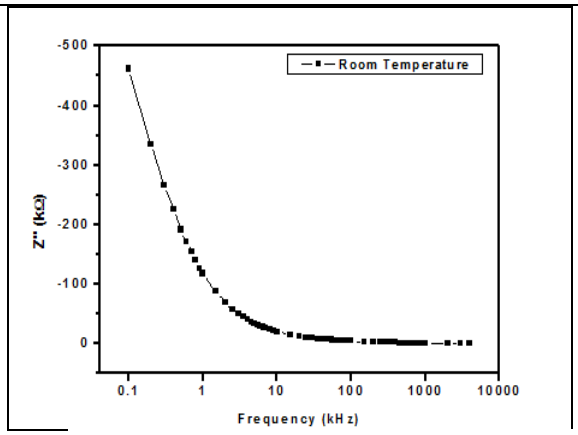

Fig.2: variation of imaginary part of impedance with frequency

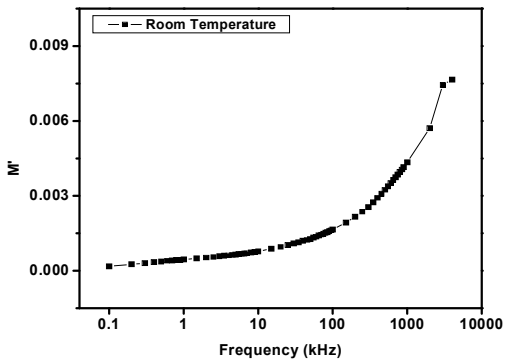

Fig.3: Variation of real part of modulus (M') with frequency

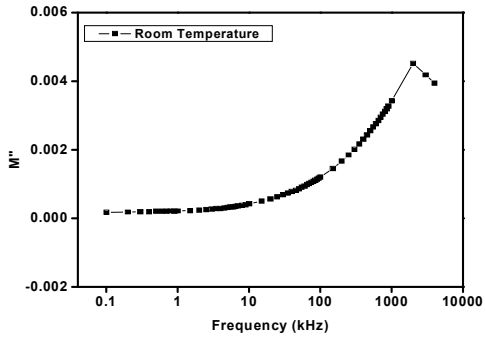

Fig.4: Variation of imaginary part of modulus (M'') with frequency

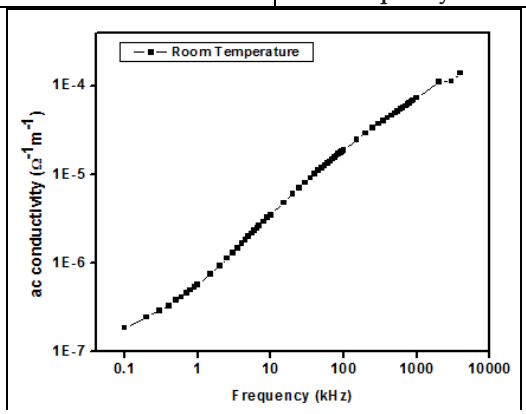

Fig.5: Variation of Conductivity as a function of frequency

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RESEARCH ARTICLE

In silico Analysis of Polyvinyl Alcohol and Polyethyl Urethane Compatibility in a Blend

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ABSTRACT

Combination of two or more components results in the formation of a blend. The compatibility ofvinyl alcohol andethylurethanewere studied to form a miscible blend using Biovia Materials Studio. The compatibility of the two components was demonstrated based on free energy of mixing, chi parameter,phase diagram andmixingenergy.The results indicated that the pair can become compatible at both low and high temperature. Phase diagram indicated that a single phase can be obtained above 387.5K which was the critical temperature. The coordination number was found to be 5.28+/-0.03. The highest number of configurations with respect to energy level was found to be-9.2kcal/mol. This study will not only help to determine pairs without performing laboratory experiments but also less time consuming and low cost process.

Keywords: Blend, *In silico*, Polyvinyl alcohol, Urethane

INTRODUCTION

Blends or composites are formed with combination of more than one component where components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisableto combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method andthis technique is a low cost and less time consuming method. Thus, researchers have focused on the use of *In silico* approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs.

Polyvinyl alcohol (PVA) is a promising material among the various polymers because of its high dielectric strength, easy film formation, adhesivity and the properties of which can be regulated by dopant concentrations [8, 9]. PVA's film forming capability is commonly used to form solid polymeric films in the packaging industryThis is due to their high mechanical strength, eco-stability and fast processing [10]. PVA is non-toxic, semi-cristalline, hydrophilic, biocompatible and easily water soluble [11].In addition, the polyethylurethane polymers were selected as α-tocopherol drug carriers.This active ingredient is widely used as a powerful antioxidant in many potential applications, including medical and cosmetic applications but is rapidly degraded due to its sensitivity to light , heat and oxygen [12]. The goal of this study is to identify the interaction between polyvinyl alcohol and polyethyl urethane in forming blends.

MATERIALS AND METHODS

Software Used: Biovia software (Dassault Systemes of France) materials studio module was used for the analysis.The software uses machine learning techniques and regular algorithms to forecast interaction rates.

Methodology: Vinyl alcohol andethylurethane were prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyvinyl alcohol was used as the base and ethylurethane was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of vinyl alcohol and ethylurethane as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where $\Delta G_m = Gibbs\ free\ energy\ of\ mixing$

$\Delta H_m = Enthalpy\ of\ mixing$

$\Delta S_m = Entropy\ of\ mixing$

T = *Absolutetemperature*

The value of $T\Delta S_m$is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$\Delta H_m < T\Delta S_m$ (2)

Figure 1 shows that the free energy involved in mixing is always negative or less than zero for the temperatures studied. The free energy decreases with increase in temperature (upto 275 K) as evident from Eq. 1 and free energy increases with increase in temperature. The results indicated that the blend will lead to ahomogenous mixture for the temperature range studied (50 to 500 K). The trend shows a very good compatibility between polyvinyl alcoholand poly ethylurethane with negative value of mixing energy,which may lead to form a particular shape with significantly high effort.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similar components may lead to a high positive value of χ (chi). Figure 2 shows that the value of x high from temperature ranging from 50Kto 500K Thevalue of x decreases exponentially with increase in temperature.This agrees with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It is assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size. In this study the coordination number was found to be 5.28+/-0.03.

Phase Diagram: The compatibility of binary mixtures can be visualized by phase diagrams. Figure 3 shows the phase diagram for the two components of the blend. There are three regions of different degree of miscibility:
a. The single-phase miscible region existed above the critical temperature of around 750 K. This value supported the fact that a single phase blend can be formed at a high temperature (higher than 750 K).
b. Fragmented metastable regions existed between binodals and spinodals, and
c. The two-phase separated regions of immiscibility are bordered by the spinodals.

The binodals separated miscible (one-phase) and metastable region, while the spinodals separated the metastable and two-phase region. When the system enters from single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e, slow nucleation followed by growth of the phase separated domains. On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distribution for Blend: The generation of different orientations using the pair's method may lead to configurations of varying energy levels. Figure 5 shows the plot of frequency (P(E)) against energy levels. This shows that the distribution is somewhat symmetrical and long chain high energy level. The number of configurations with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -2.00 kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 5 shows that the mixing energy for the system was small for the temperature range studied. The graph indicated that at first when temperature increases the mixing energy increases to a highest value after that when again temperature increases the mixing energy becomes decreases and again further increases with increase in temperature.The temperature is vary from 50K to500K for the varying of mixing energy.it is very much possible to mix the two components at any feasible temperature with least mixing energy value.

CONCLUSION

The possibility of use of polyvinyl alcohol and ethyl urethane to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair can have very good compatibility at different ranges of temperature. The coordination number was found 8.25+/-0.03. The maximum number of configurations with respect to energy level was found to -9.2Kcal/mol.Usually components for a blend is identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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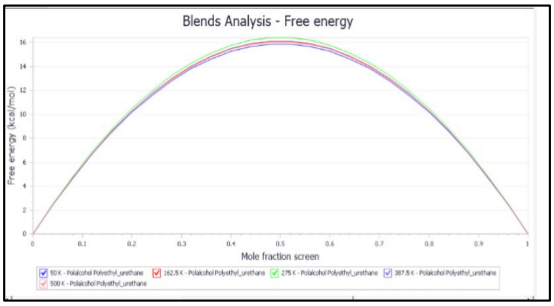

Figure 1. Free energy change with mole fraction of polyethylurethane at different temperatures

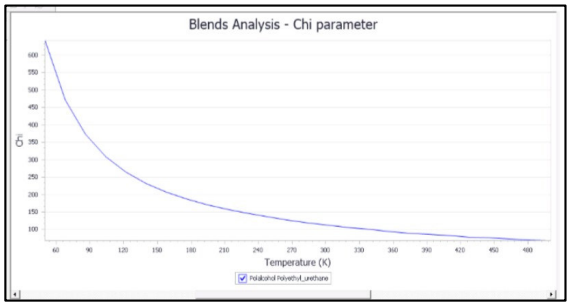

Figure 2. Change in χ (chi) value with temperature

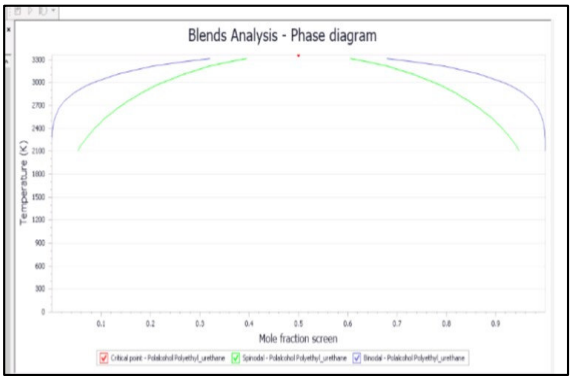

Figure 3. Phase diagram

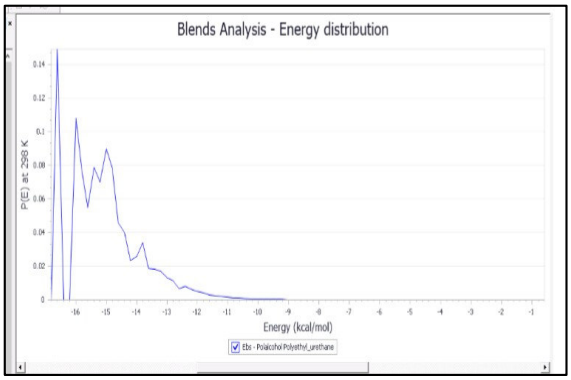

Figure 4. Energy distribution

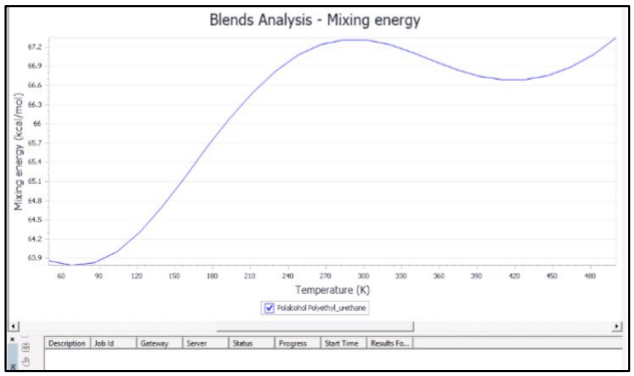

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyvinyl Alcohol and Polyoxyethylene Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all those parameters increased with increase in mass fraction of vinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Blend, *In silico*, Polyvinyl alcohol, Polyoxyethylene composite

INTRODUCTION

Blends or composites are materials containing more than one components. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials[3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio

and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of *In silico* approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Further, PVA (polyvinyl alcohol) is an essentialpolymeric material which is universally benefitedin packaging industry to form strong polymeric materials and excellent film forming natures. because of itseasy formation of film, high dielectric strength,high mechanical strength, high thermal conductivity, stability of environment andadhesiveness etc. These properties of material can be fluctuated by various contentof dopant [8-10]. Meanwhile, the PVA is non-toxic, semi-crystalline, hydrophilic, biocompatible and easily soluble in water [11]. Furthermore, a molecular complexof high-molecular polyoxyethelene-urea mixtureswith respect to thermal behavior in between 20^0-500°Cwas explored by means of a derivatograph.This study is intended to identify the conversion of polyvinyl alcohol into a sponge-like material by foaming agents and hardened with formaldehyde and polyoxyethelene to form blends [12-13].

MATERIALS AND METHODS

Software Used

The software used for analysis was Materials studio module of Biovia (France Dassault Systemes). The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

The structures of polyvinyl alcohol and polyoxyethelene were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS & DISCUSSION

In this work the use of polyvinyl alcohol and polyoxyethelene as potential components of a composite was analyzed using BIOVIA Materials Studio which needs pre-defined correlations (advanced quantitative structure-property relationships) to figure out a broad range of polymer properties. The methods of Group additive were operated for many years to predict the properties of small molecules and polymers. For extremely fast property estimation without detailed knowledge of the atomistic interactions, these methods are of greatest utility and easy to operate. However, the principal drawback of these methods is the dependence upon the database of group contributions. Thus, without group contribution database the property of polymer cannot be determined.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, properties ofany polymer may be predicted without database of group contributions by the composition of any combination of the following nine elements: hydrogen(H), carbon(C), nitrogen(N), oxygen(O),bromine(Br), silicon(Si), sulfur(S), fluorine(F), chlorine(Cl).

Heat capacity: It is the amount of heat required without change of phase to raise the temperature of one-unit weight of a substance by 1°C. Figure 1 shows that the heat capacity (Cp) of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Thermal conductivity: It indicates the correlation between heat flux per unit area and temperature gradient. It refers to the intrinsic ability of a material to transfer heat. Figure 2 shows that the thermal conductivity of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Dielectric constant: It is defined as the ratio of the electric permeability of the material to the electric permeability of free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant. Figure 3 shows that the dielectric constant of the composite increases with increase in mass fraction of vinyl alcohol.

CONCLUSION

The possibility of use of polyvinyl alcohol and polyoxyethelene to form a blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all the three parameters increased with increase in mass fraction of vinyl alcohol. Usually components for a blend are identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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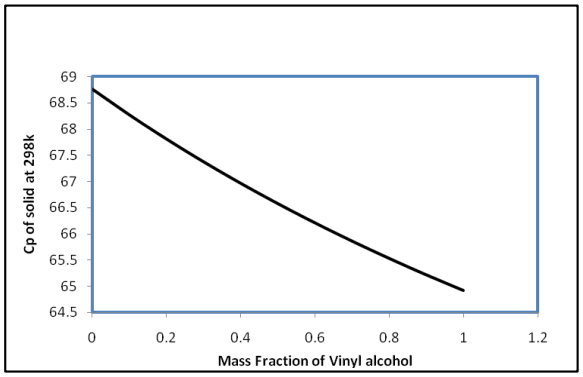

Figure 1. Change in heat capacity with mass fraction of vinyl alcohol

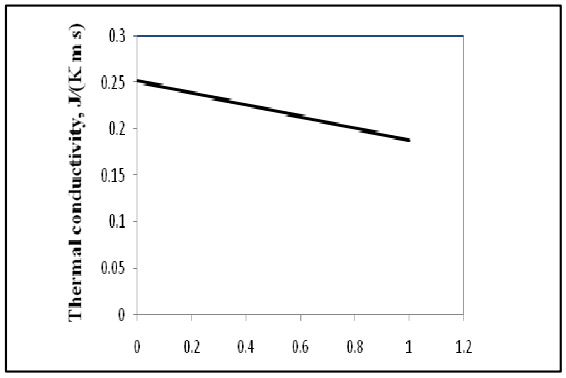

Figure 2. Change in thermal conductivity with mass fraction of vinyl alcohol

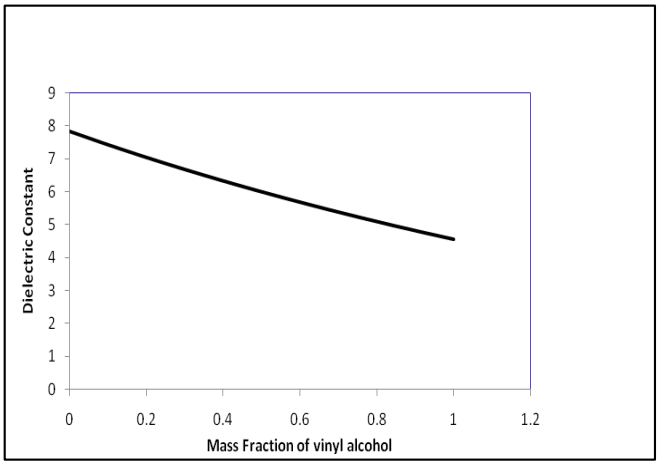

Figure 3. Change in dielectric constant with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyvinyl Alcohol and Polyethylur ethane Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all those parameters increased with increase in mass fraction of Vinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Blend, *In silico*, Polyvinyl Alcohol, Polyethylurethane composite

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were

developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of *In silico* approach to develop new blends. Software (Materials Studio [7] have been used to identify compatible pairs. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. Due to extreme mechanical strength, eco friendly and easy fabrication process of PVA, it is mostly used in packaging industry to make strong polymeric film [8]. It also attracts the researcher because of its some excellent characteristics like semi-crystalline, hydrophilic, biocompatible and easily soluble in water [9]. Ethylurethane can be combined with other materials for drug delivery for α-tocopherol. It is also applicable in area of medicine and cosmetic as a strong antioxidant. Their application is limited due to its fast degrading nature because of environmental sensitivity [10]. So the objective of the work is to manifest the interaction of polyvinyl alcohol and polyethyl urethane to form blends.

MATERIALS AND METHODS

Software Used: Analysis was done by a software "Materials studio module of Biovia" (Dassault Systemes of France). The interaction level is predicted using machine learning techniques and standard algorithms of the software.

Techonic: The structures of Vinyl alcohol and ethylurethane were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of Vinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of Vinyl alcohol and ethylurethane as potential components of a composite was analyzed using "Biovia Materials Studio". "BIOVIA Materials Studio Synthia" uses preset connections (advanced quantitative structure-property relationships) to work out various characteristics of polymer. Earlier the properties of polymers and small molecules were estimated by group additive methods because of its simplicity and rapidness. But this technique suffers from certain drawbacks as it requires a large database. So the polymers of specific group can be characterized by this method.

So to study unknown polymers and its interaction with other materials Synthia method is adopted for topological information. The dependent parameters obtained from graph theory are shown. So a specific group contributions is not necessary for combination of a polymer with any following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Heat capacity: The thermal energy required to increase the temperature of unit mass of a substance by 1°C at a given phase is known as heat capacity. Figure 1 shows that the heat capacity (Cp) of the composite increases linearly with increase in mass fraction of Vinyl alcohol.

Thermal conductivity: It indicates the correlation between heat flux per unit area and temperature gradient. It refers to the intrinsic ability of a material to transfer heat. Figure 2 shows that the thermal conductivity of the composite increases linearly with increase in mass fraction of Vinyl alcohol.

Dielectric constant: Dielectric constant is the fraction of increase of bound charges in the medium as compared to free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant. Figure 3 shows that the dielectric constant of the composite increases with increase in mass fraction of vinyl alcohol.

CONCLUSION

The possibility of use of polyvinyl alcohol and polyethylurethane to form a blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all the three parameters increased with increase in mass fraction of Vinyl alcohol. Usually components for a blend are identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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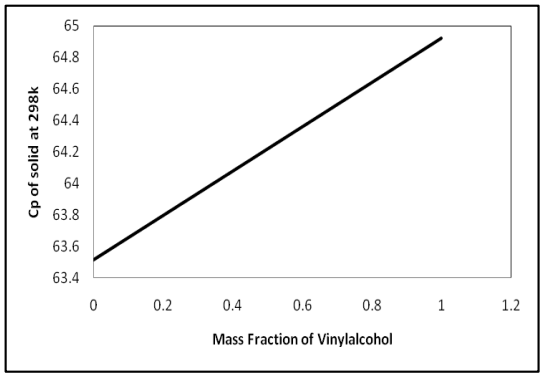

Figure 1. Change in heat capacity with mass fraction of ethylurethane

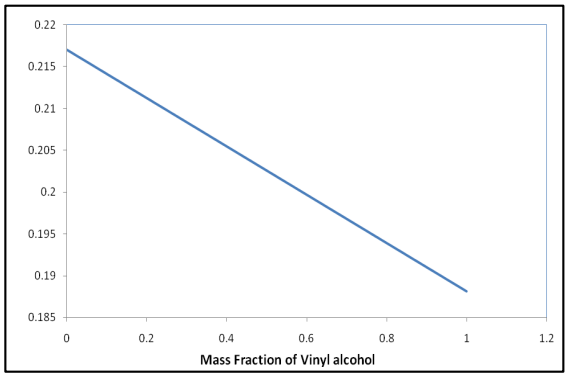

Figure 2. Change in thermal conductivity with mass fraction of vinylalcohol

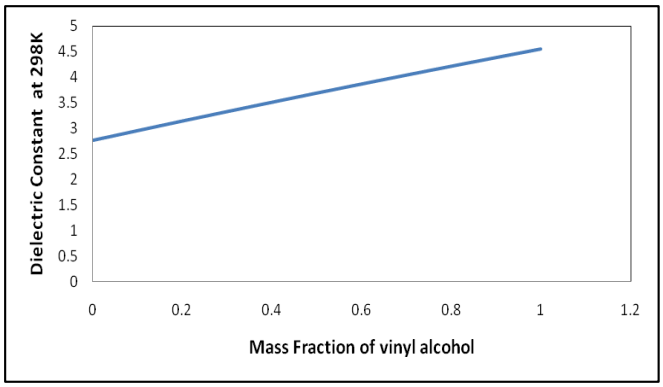

Figure 3. Change in dielectric constant with mass fraction of vinylalcohol

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyvinyl Alcohol and Polyurea Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all those parameters increased with increase in mass fraction of Vinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Blend, *In silico*, Polyvinyl Alcohol, Poly urea composite

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials[3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were

developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of *In silico* approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.For dental implants, anddenture bases, dental repairmen, and for various skeletal defects Polyvinyl alcohol polymers are largely used [8, 9]. They are also used as dispersing agent, superabsorbent polymer, ion-exchange resin, etc.[10]. Moreover, these polymers have easy processing, low cost and wide variety of applications in the field electrical and electronic components. Polyvinyl alcoholis a polyelectrolyte soluble in aqueous media at neutral pH. It is used for preparing hydrogels. It is not toxic and does not cause irritation [11].

Researchers have used polyurea in combination with other materials to act as adsorbent [12]. Inaddition, the polyurea have elastomeric thermoset polymeric materials and has various new fields of militaryapplications because of its high mechanical strength [13]. This study is intended to identify the interaction of polyvinyl alcoholand polyurea to form blends.

MATERIALS AND METHODS

Software Used: The software "Materials studio module of Biovia" (DassaultSystemes of France) was adopted for analysis purpose. The interaction between different materials is studied via machine learning techniques and standard algorithms.

Working: The structures of polyvinyl alcoholandpolyurea were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcoholon the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of Vinyl alcohol and ethylurethane as potential components of a composite was analyzed using "Biovia Materials Studio". "BIOVIA Materials Studio Synthia" uses preset connections (advanced quantitative structure-property relationships) to work out various characteristics of polymer.The conventional technique to study the polymer properties and its combination was group additive methods which was quite simple and fast process.But this technique has a big shortcoming that it requires a particular database for each component which is another difficult task..

.So the appropriate answer to the above difficulties is Synthia method for proper topological information.Again graph theory plays an important role along with the software to study unknown polymers and its interaction with other materials.So a polymer belongs to any group can combine with the given elements : carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine to form a composite.

Heat capacity: The energy supplied to increase the temperature of unit mass of the substance through unit range is called heat capacity**.** It is the amount of heatrequired to raise the temperature of one unit weight of a substance by 1°C without change of phase.Figure 1 shows that the heat capacity (Cp) of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Thermal conductivity: It indicates the correlation between heat flux per unit area and temperature gradient.It refers to the intrinsic ability of a material to transfer heat.Figure 2 shows that the thermal conductivity of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Dielectric constant: The relative permittivity of a material with respect to air is the dielectric constant.. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant.Figure 3 shows that the dielectric constant of the composite increases with increase in mass fraction of vinyl alcohol.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly urea to form a blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all the three parametersincreased with increase in mass fraction of vinyl alcohol. Usually components for a blend are identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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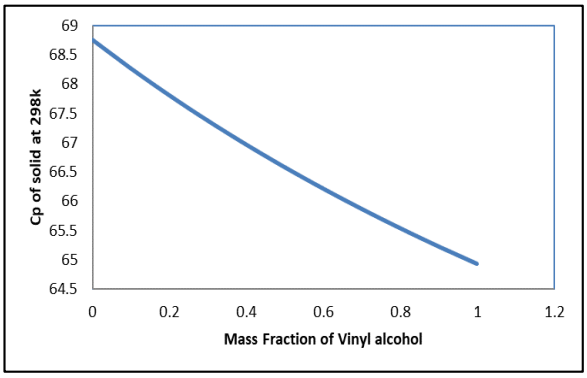

Figure 1. Change in heat capacity with mass fraction of vinyl alcohol.

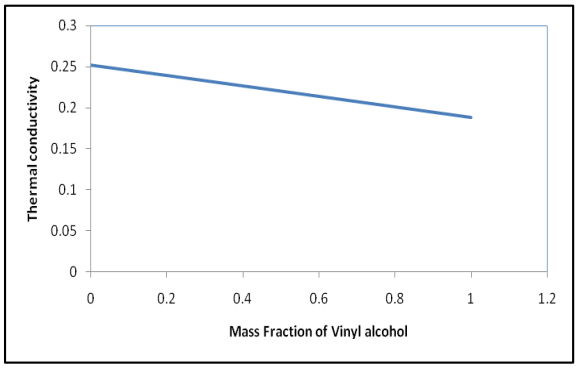

Figure 2. Change in thermal conductivity with mass fraction of vinyl alcohol.

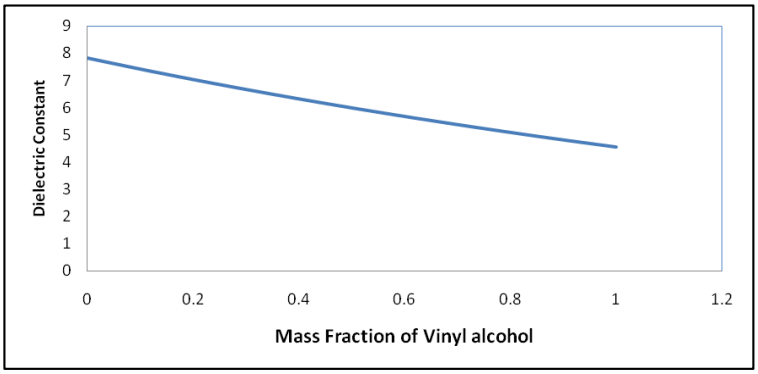

Figure 3. Change in dielectric constant with mass fraction of vinyl alcohol.

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyvinyl Alcohol and Polyethyl Urethane Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of polyvinyl alcohol and polyethyl urethane to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in polyvinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases decreased with increase in mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Blend, *In silico*, Polyvinyl Alcohol, Polyethyl urethane composite

INTRODUCTION

Blends or composites are materials containing more than one components. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance

flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementations composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of *In silico* approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by do pant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy process ability [10]. On the other hand, PVA is non-toxic, semi-crystalline, hydrophilic, biocompatible, excellent water soluble and better film forming ability [11].

However, the polyethylurethane polymers were chosen as drug carriers for α-tocopherol. This active ingredient is widely used as a strong antioxidant in many potential applications including medical and cosmetic, but is rapidly degraded, because of its light, heat and oxygen sensitivity [12]. This study is intended to identify the interaction of polyvinyl alcohol and poly ethyl urethane to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and polyethyl urethane were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and polyethyl urethane as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of

group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar Volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite decreases linearly with increase in mass fraction of polyethyl urethane.

Density: Increase in density indicates decrease in porosity. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite decreases linearly with increase in mass fraction of polyethyl urethane.

Permeability of Gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium.Lower permeability indicates longer time lag for the gas to pass through the mebrane. Figure 3 show that the permeability of oxygenthrough the composite decreases with increase in mass fraction of polyethyl urethane.

Figure 4 show that the permeability of nitrogenthrough the composite decreases with increase in mass fraction of acrylic acid. Figure 5 show that the permeability of carbon dioxidethrough the composite decreases with increase in mass fraction of acrylic acid. Thus the results indicated that an increase in acrylic acid fraction reduces the permeability of different gases. The rate of permeability might be influence by the molecular weight of the gases.

CONCLUSION

The possibility of use of polyvinyl alcohol and polyethyl urethane to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties.The molar volume and density decreased with increase in acrylic acid fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeabilityfor all the gases decreased with increase in mass fraction of acrylic acid. Usually components for a blend are identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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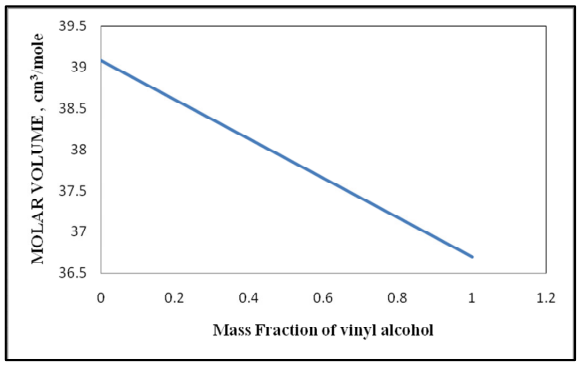

Figure 1. Change in molar volume with mass fraction of vinyl alcohol

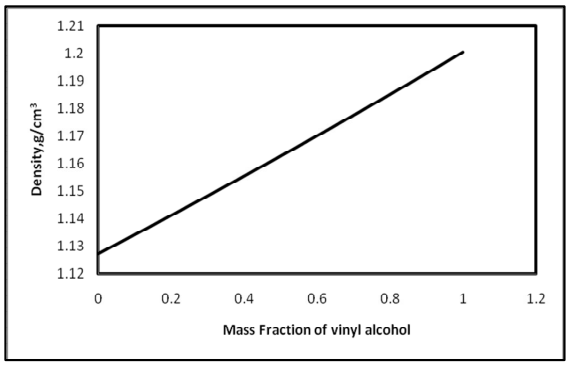

Figure 2. Change in density with mass fraction of vinyl alcohol

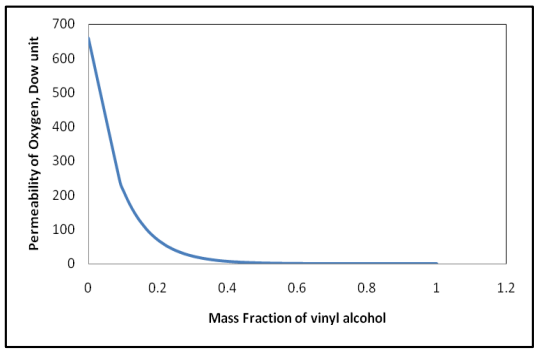

Figure 3. Change in permeability of oxygen with mass fraction of polyethyl urethane

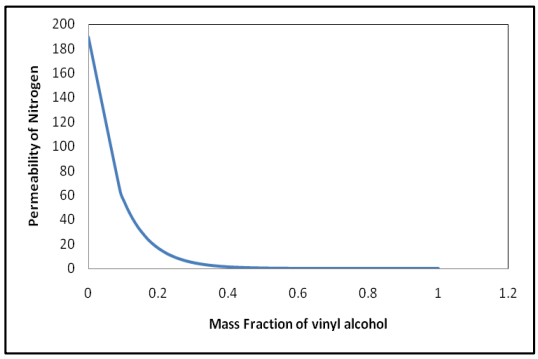

Figure 4. Change in permeability of nitrogen with mass fraction of polyethyl urethane

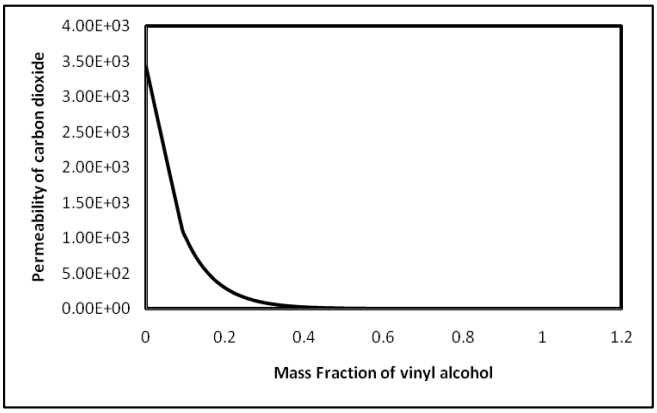

Figure 5. Change in permeability of carbon dioxide with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyvinyl Alcohol and Polyoxymethylene Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of polyvinyl alcohol and Polyoxymethylene to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in polyvinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases decreased with increase in mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Blend, *In silico*, Polyvinyl Alcohol, Polyoxy methylene composite

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of

lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of *In silico* approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs.

Among the various polymers, polyvinyl alcohol is a promising material [8, 9]. The film forming ability of polyvinyl alcohol is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, polyvinyl alcohol is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11]. Researchers have used Polyoxymethylene in combination with polyvinyl alcohol based materialsshows good permeability behaviour. The radiochemical degradation of a "polyoxymethylene homopolymer (POM)" was used to study the effects of molar mass changes in the crystalline structure [12-13]. The properties are intended to identify the interaction of polyvinyl alcohol and polyoxymethylene to form blends.

MATERIALS AND METHODS

Software Used: "Materials studio module of Biovia software (Dassault Systemes of France)" was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and Polyoxymethylene were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcoholon the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and polymerX as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in "Synthia" uses topological information about polymers in the predictive correlations. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite decreases linearly with increase in mass fraction of vinyl alcohol

Density: Increase in density indicates decrease in porosity. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite decreases linearly with increase in mass fraction of vinyl alcohol

Permeability of gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium. Lower permeability indicates longer time lag for the gas to pass through the membrane. Figure 3 shows that the permeability of oxygen through the composite decreases with increase in mass fraction of vinyl alcohol

Figure 4 shows that the permeability of nitrogen through the composite decreases with increase in mass fraction of vinyl alcohol. Figure 5 shows that the permeability of carbon dioxide through the composite decreases with increase in mass fraction of vinyl alcohol. Thus the results indicated that an increase in vinyl alcohol fraction reduces the permeability of different gases. The rate of permeability might be influence by the molecular weight of the gases.

CONCLUSION

The possibility of use of polyvinyl alcohol and Polyoxy methylene to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in vinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeability for all the gases decreased with increase in mass fraction of vinyl alcohol usually components for a blend are identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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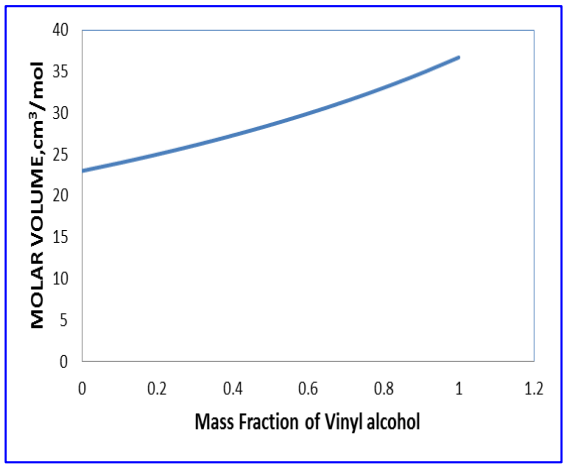

Figure 1. Change in molar volume with mass fraction of vinyl alcohol

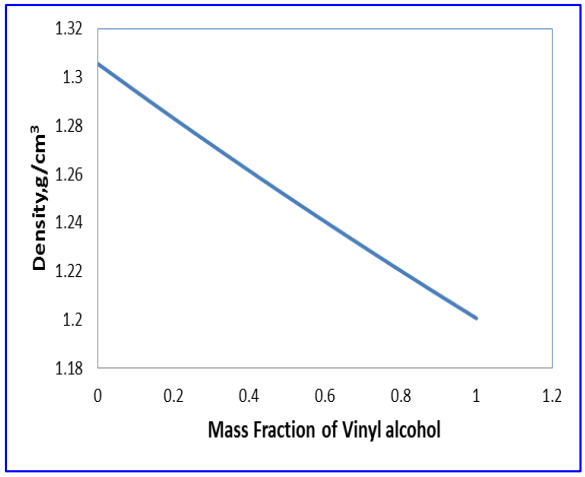

Figure 2. Change in density with mass fraction of vinyl alcohol

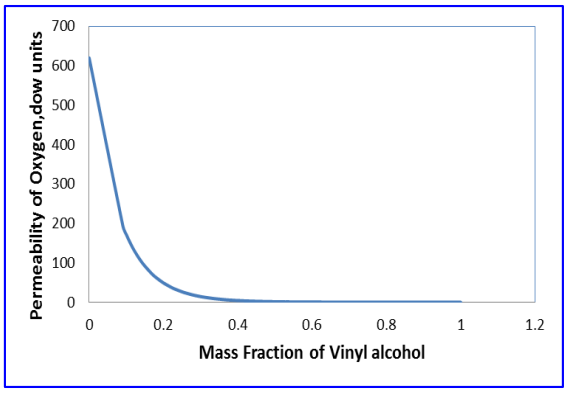

Figure 3. Change in permeability of oxygen with mass fraction of vinyl alcohol

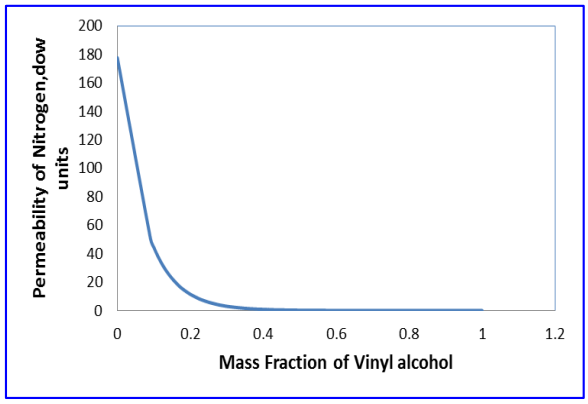

Figure 4. Change in permeability of nitrogen with mass fraction of vinyl alcohol

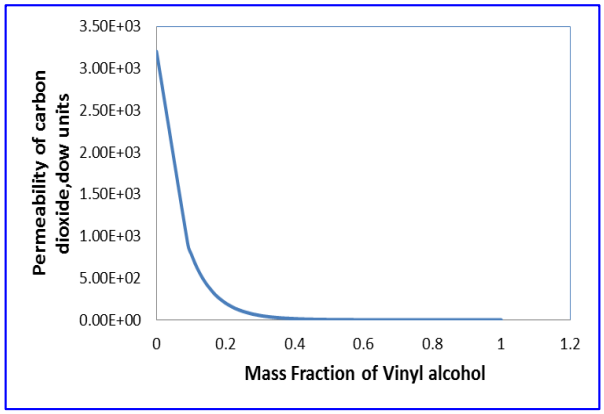

Figure 5. Change in permeability of carbon dioxide with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyacrylic Acid and Polyacrylonitrile Composite

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Received: 18 Mar 2020 Revised: 21 Apr 2020 Accepted: 22 May 2020

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ABSTRACT

Generally blend is a mixture of more than one components and the desired property is its homogeneity. In this current article the composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results signify that all those parameters increased with increase in mass fraction of acrylic acid. This study will help the researchers for determining the pairs of component of blend without laboratory experiment performance which save materials, money as well as time.

Keywords: Blend, *In silico*, Polyacrylic Acid and Polyacrylonitrile Composite

INTRODUCTION

Blends or composites are materials containing more than one components. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of

transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of *In silico* approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Acrylic polymers shows wide range of applications in maxillofacial appliances for skeletal defects etc. [8], bone repair [9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc.[10]. Polyacrylic acid is used as a electrolyte soluble in aqueous media at neutral pH, good adsorbent, hydrophobic, biocompatible and used as electrolyte [11, 12]. Researchers have used "polyacrylonitrile (PAN)" is a carbon fiber precursor and is also used for activated carbon. This study is intended to identify the interaction of polyacrylic acid and polyacrylonitrile to form blends.

MATERIALS AND METHODS

Software Used: "Materials studio module of Biovia software (Dassault Systemes of France)" was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyacrylic acid and polyacrylonitrile were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyacrylic acid on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acid and polyacrylonitrile as potential components of a composite was analyzed using "Biovia Materials Studio". BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated. To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed.

Heat capacity: Figure 1 shows that the heat capacity (Cp) of the composite increases linearly with increase in mass fraction of acrylic acid.

Thermal conductivity: It indicates the correlation between heat flux per unit area and temperature gradient. It refers to the intrinsic ability of a material to transfer heat. Figure 2 shows that the thermal conductivity of the composite increases linearly with increase in mass fraction of acrylic acid.

Dielectric constant: Figure 3 shows that the dielectric constant of the composite increases with increase in mass fraction of acrylic acid.

CONCLUSION

The possibility of use of polyacrylic acid and polyacrylonitrile to form a blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all the three parameters increased with increase in mass fraction of acrylic acid. Usually components for a blend are identified experimentally. This *In silico* study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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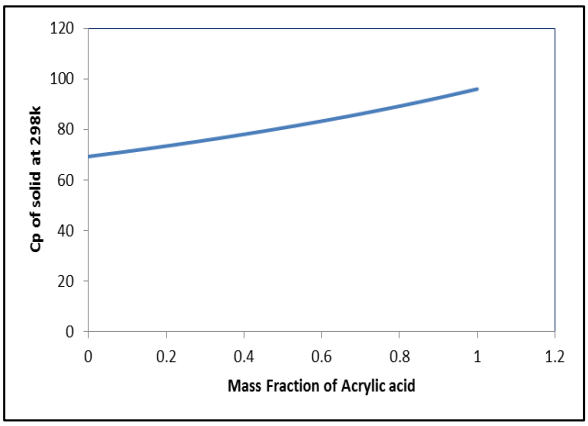

Figure 1. Change in heat capacity with mass fraction of acrylic acid

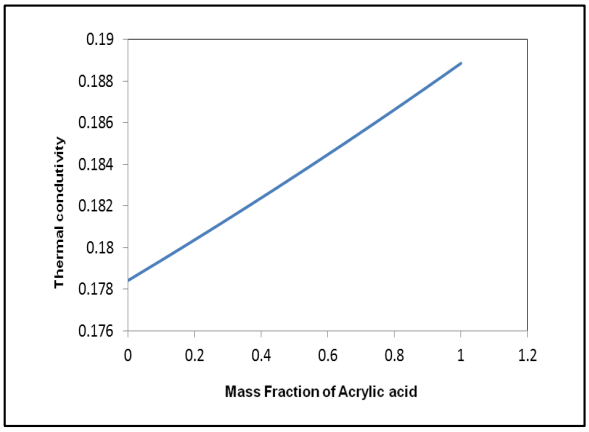

Figure 2. Change in thermal conductivity with mass fraction of acrylic acid

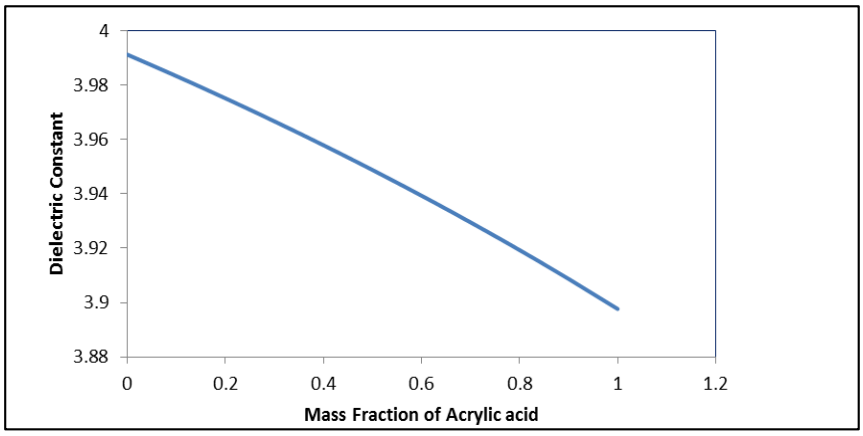

Figure 3. Change in dielectric constant with mass fraction of acrylic acid

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyacrylic Acid and Polyacrylochloride Composite

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ABSTRACT

A blend may be a mixture of more than one component. The specified property of a mix is its homogeneity. The composition of polyacrylic acid and polyacrylochloride to supply desired mechanical properties of the blend was explored using Bio via Materials Studio. The mechanical properties of the composite were studied supported bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle fatigue fracture. The results indicated that the values of all the properties increased with increase in mass fraction of propanoic acid. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: blend, polyacrylic acid, polyacrylochloride, mechanical properties

INTRODUCTION

Blends or composites are materials containing quite one component. The components don't lose their identity within the mixture. They combine and contribute to the property of the blend thereby improving the standard of the fabric. Development of one material with the specified property involves significant research and time. a mix utilizes the benefits of various materials, mix them to urge the specified property. Thus, a mix saves time to develop a replacement material thereby reducing the value of development of products with desired properties. Polymer blends are often made from two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the thanks to multi-functional materials. Polymers including carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] are reported to reinforce mechanical properties and water resistance. Researchers are performing on

fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; which will enhance flame retardancy without increasing the load [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency within the field of transportation [5]. There are applications of composites in structural Engineering thanks to high strength to weight ratio and resistance to corrosion. Thus, optical fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above-mentioned examples relied on laboratory experiments.Usually blends are prepared by trial and error method. Thus, it involves wastage of materials, time and money. Thus, researchers have focused on the utilization of in silico approach to develop new blends. Software (Materials Studio [7]) are wont to identify compatible pairs.Acrylic polymers have an honest kind of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects etc. [8], bone repair [9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc. [10]. Polyacrylic acid may be a polyelectrolyte soluble in aqueous media at neutral pH it's used for preparing hydrogels. it's not toxic and doesn't cause irritation [11].Researchers have used polyacrylochloride together with other materials to act as adsorbent [12]. Polyacrylochloride are reported to be utilized in Curtius reaction.This study is meant to spot the interaction of polyacrylic acid and polyacrylochloride to make blends.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systems of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the extent of interaction.

Methodology

The structures of polyacrylic acid and polyacrylochloride were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyacrylic acid on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the utilization of polyacrylic acid and polyacrylochloride as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to gauge a good range of polymer properties. Group additive methods were used for several years to predict the properties of polymers also as small molecules. These methods are extremely fast and straightforward to use. Consequently, they're of greatest utility when a rapid estimate of a property is required without an in depth understanding of the atomistic interactions that produce thereto. However, the principal shortcoming of those methods is their dependence upon a database of group contributions. Thus, if a polymer contains a gaggle that the group contribution cannot be estimated, then the property of that polymer cannot be calculated.To overcome this limitation, the tactic implemented in Synthia uses topological information about polymers within the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties could also be predicted for any polymer composed of any combination of the subsequent nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Bulk modulus: coefficient of elasticity is that the measure of the decrease in volume with a rise in pressure. Figure 1 shows that the majority modulus of the composite increases linearly with increase in mass fraction of acrylic acid.

Shear modulus: It is defined because the ratio of shear stress and shear strain. It shows the response of the composite to shear deformation. Figure 2 shows that the shear modulus of the composite increases linearly with increase in mass fraction of acrylic acid.

Young's modulus: It is defined because the ratio of stress and strain. It compares the relative stiffness of the composite. Figure 3 shows that the Young's modulus of the composite increases linearly with increase in mass fraction of acrylic acid.

Poisson ratio: It is the ratio of lateral strain to longitudinal strain. Figure 4 shows that the Poisson ratio of the composite increases linearly with increase in mass fraction of acrylic acid.

Brittle fracture stress: Brittle Fracture is the abrupt, rapid cracking of a materialbelow stress where the material displayedpractically no sign of ductility or plastic degradation before the fracture happens. Figure 5 shows that the brittle fracture stress of the composite growths linearly with growth in mass fraction of acrylic acid.

CONCLUSIONS

The possibility of use of polyacrylic acid and polyacrylochloride to make a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with reference to mechanical properties. The mechanical properties of the composite were studied supported bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle fatigue fracture. The results indicated that the values of all the properties increased with increase in mass fraction of acrylic acid. Usually components for a mix are identified experimentally. This in silico study will help determine components of a mix without performing laboratory experiments saving materials, money and time.

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12. Chromatographic Separation of As(DI), Sb(III) and Bi(HI) with Poly Calix-crown Hydroxamic Acid.

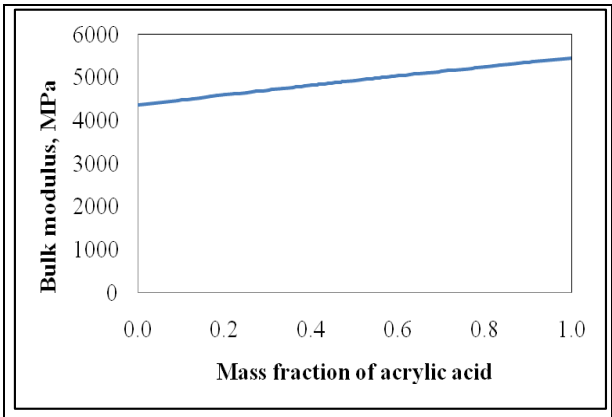

Figure 1. Change in bulk modulus with mass fraction of acrylic acid

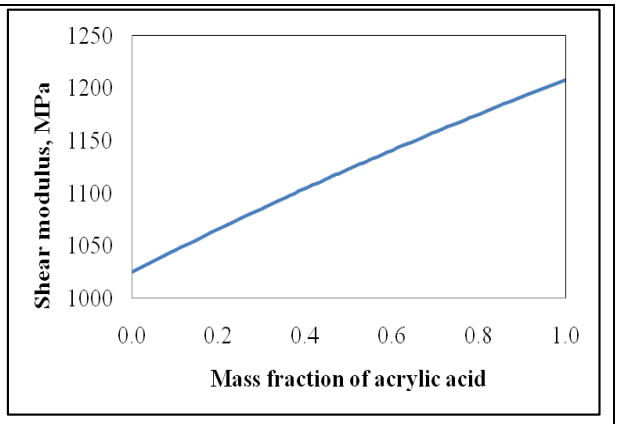

Figure 2. Change in shear modulus with mass fraction of acrylic acid

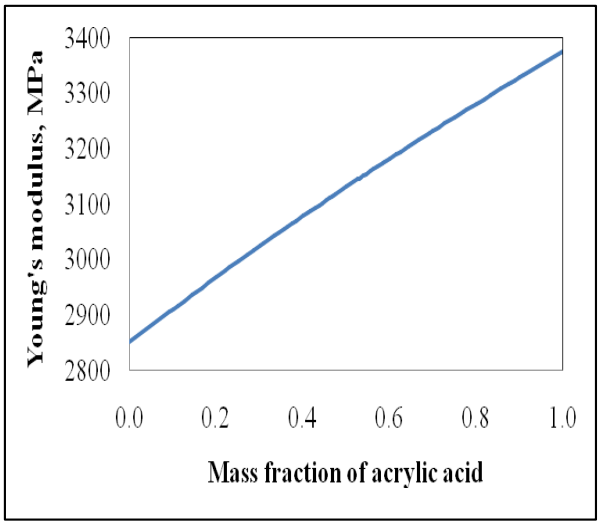

Figure 3. Change in Young's modulus with mass fraction of acrylic acid

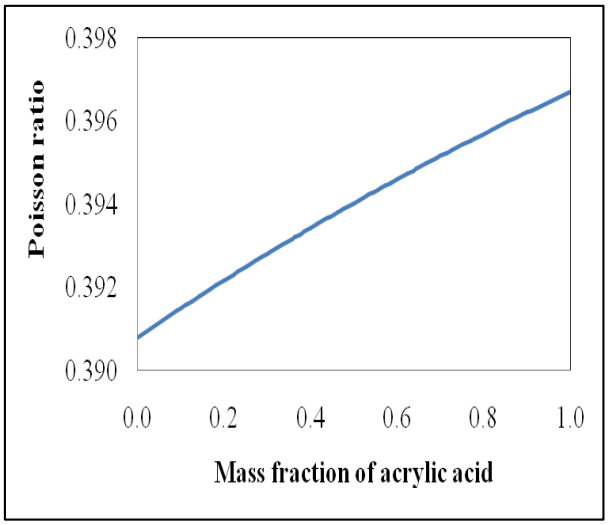

Figure 4. Change in Poisson modulus with mass fraction of acrylic acid

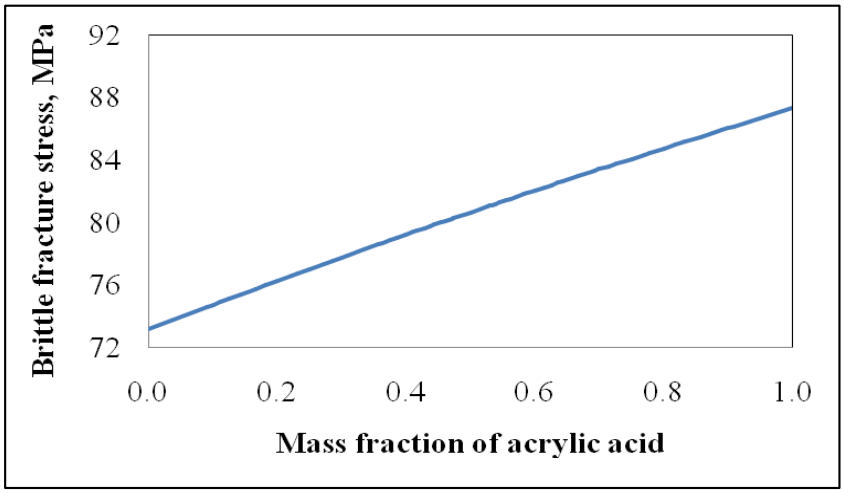

Figure 5. Change in brittle fracture stress with mass fraction of acrylic acid

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RESEARCH ARTICLE

In silico Analysis of Polyacrylic Acid and Polybutylene isopthalate Compatibility in a Blend

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ABSTRACT

A blend is a mixture of more than one components.The desired property of a blend is its homogeneity. The selection of polyacrylic acid and polybutylene isopthalate to form a miscible blend was explored using Biovia Materials Studio. The compatibility of the two components was studied based on free energy of mixing, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible only at high temperature. Phase diagram indicated that a single phase can be obtained above 1000 K which was the critical temperature. The coordination number was found to be 8.51 +/- 0.05. The highest number of configurations with respect to energy level was found to be -1.4 kcal/mol. The phase separation might lead to its use as porous material to be used as adsorbent. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: blend, homogeneity, polyacrylic acid , polybutylene isopthalate, Biovia Materials Studio.

INTRODUCTION

Blends or composites are materials containing more than one components. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working

on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.Acrylic polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects etc. [8], bone repair [9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc. [10].

Polyacrylic acid is a polyelectrolyte soluble in aqueous media at neutral pH. It is used for preparing hydrogels. It is not toxic and does not cause irritation [11]. Researchers have found polybutylene isopthalate to be partially crystalline, during copolymerization and there was a lowering in the amount of crystallinity and a decrease of melting temperature with respect to pure homopolymers [12]. This study is intended to identify the interaction of polyacrylic acid and polybutylene isopthalate to form blends.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

Polyacrylic acid and polybutylene isopthalate were prepared using the build menu of Materials Studio. The structure of the components was optimized using the components used in blends->calculation menu of Materials studio. Polyacrylic acid was used as the base and polybutylene isopthalate was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acid and polybutylene isopthalate as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where ΔG_m – *Gibb's free energy of mixing*

ΔH_m = *Enthalpy of mixing*

ΔS_m = *Entropy of mixing*

T = *Absolute temperature*

The value of $T\Delta S_m$ is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$$\Delta H_m < T\Delta S_m \quad (2)$$

Figure 1 shows that the free energy involved in mixing is always positive for the temperatures studied. The free energy decreases with increase in temperature as evident from Eq. 1. The results indicated that the blend will not lead to a homogeneous mixture for the temperature range studied (50 to 500 K). The trend suggested that there might be a possibility of a miscible blend at very high temperature.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similar components may lead to a high positive value of χ (chi).
Figure 2 shows that the χ value is high for the temperature range studied (50 to 500 K) indicating demixing. The χ value decreased with increase in temperature. Thus at high temperature there is a possibility to form a miscible blend. The result is in agreement with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size. In this study the coordination number was found to be 8.51 +/- 0.05.

Phase Diagram: The compatibility of binary mixtures can be visualized by phase diagrams. Figure 3 shows the phase diagram for the two components of the blend. There are three regions of different degree of miscibility:

a. The single-phase miscible region existed above the critical temperature of around 1000 K. This value supported the fact that a single phase blend can be formed at a high temperature (higher than 1000 K).
b. Fragmented metastable regions existed between binodals and spinodals, and
c. The two-phase separated regions of immiscibility are bordered by the spinodals.

The binodals separated miscible (one-phase) and metastable region, while the spinodals separated the metastable and two-phase region.When the system enters from single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e, slow nucleation followed by growth of the phase separated domains. On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 4 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations

with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -1.4 kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 5 shows that the mixing energy for the system was high for the temperature range studied. The graph indicated that an increase in temperature increased the mixing energy .The formation of nonhomogeneous blend with polyacrylic acid as base might help formation of blend with higher porosity such as hydrogel. This might have an application as adsorbent.

CONCLUSIONS

The possibility of use of polyacrylic acid and polybutylene isopthalate to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible at high temperature. Phase diagram indicated that a single phase can be obtained above 1000 K. The coordination number was found to be 8.51 +/- 0.05. The maximum number of configurations with respect to energy level was found to be -1.4 kcal/mol. The phase separation might make it a porous material to be used as an adsorbent. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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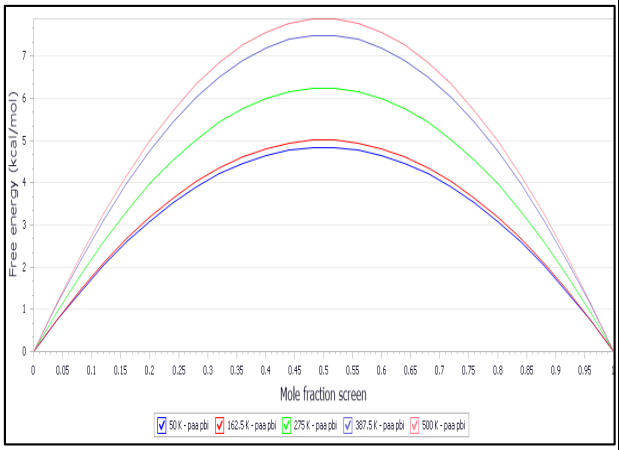

Figure 1. Free energy change with mole fraction of polybutylene isopthalate at different temperatures

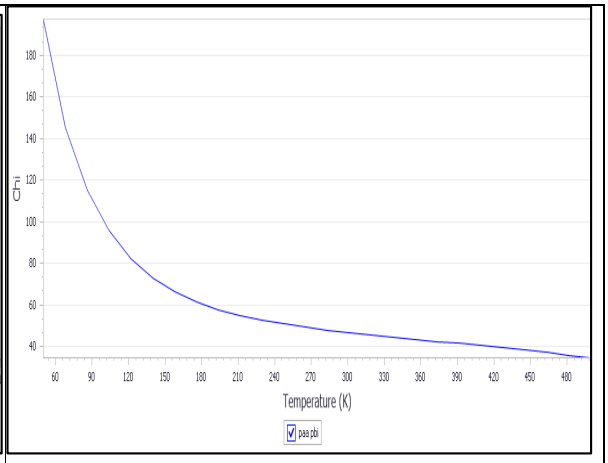

Figure 2. Change in χ (chi) value with temperature

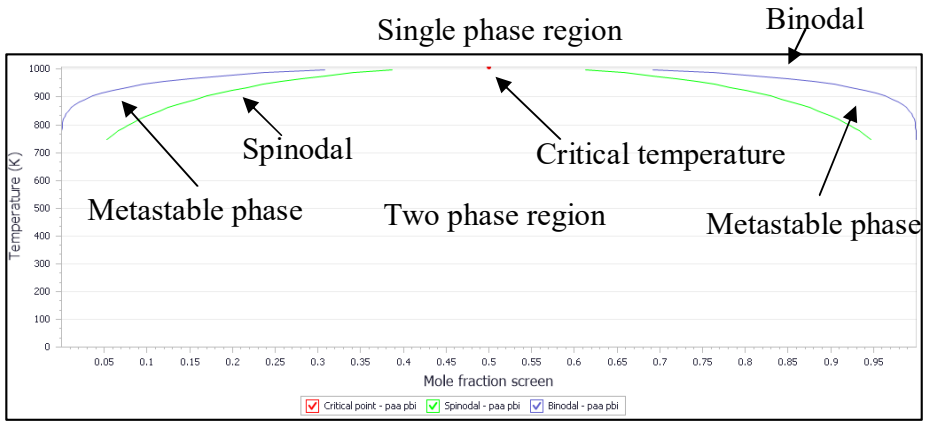

Figure 3. Phase diagram

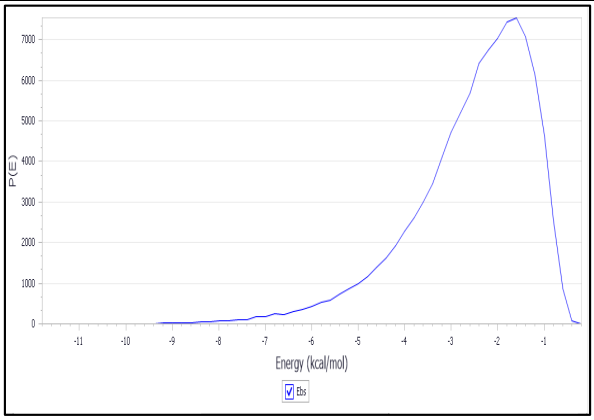

Figure 4. Energy distribution

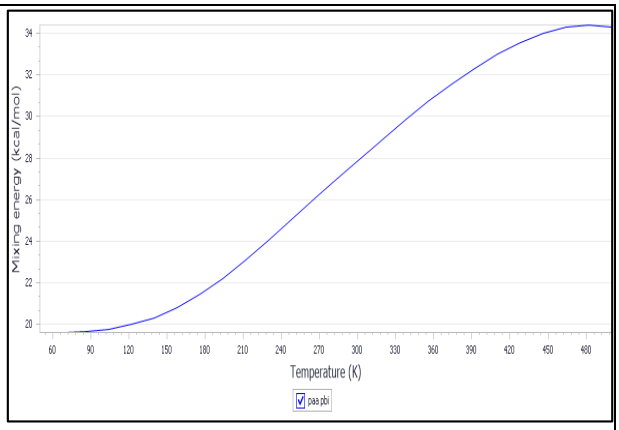

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyacrylic Acid and Poly12a D Glucose Compatibility in a Blend

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ABSTRACT

A blend is always a composition of two or more components and it is desirable to have homogeneity in a blend. In this paper, we have tried to explore the compatibility of polyacrylic acid and poly12aDglucose to form a miscible blend using Biovia Materials Studio. The compatibility of the two components was studied based on free energy of mixing, chi parameter, and mixing energy. The results indicated that the pair can have very good compatibility at low to high temperature without any phase separation. The coordination number was found to be 6.46 +/- 0.04. The highest number of configurations with respect to energy level was found to be -1.9 kcal/mol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: blend, Biovia Materials Studio, poly12a D glucose,

INTRODUCTION

Blends or composites are materials containing more than one component. The components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisable to combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength

important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.Acrylic polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects etc. [8], bone repair [9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc. [10].

Polyacrylic acid is a polyelectrolyte soluble in aqueous media at neutral pH It is used for preparing hydrogels. It is not toxic and does not cause irritation [11]. Researchers have found applications of glycopolymers (synthetic polymers containing pendant carbohydrate groups) in the separation and removal of toxins and bacteria, tumor cell recognition and glucose-responsive insulin delivery [12]. It has been found that biopolymer blends possess good thermal stability [13].This study is intended to identify the interaction of polyacrylic acid and poly12aDglucose to form blends.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

Polyacrylic acid and poly12aDglucose were prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyacrylic acid was used as the base and poly12aDglucose was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acid and poly12aDglucose as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where $\Delta G_m = Gibb's\ free\ energy\ of\ mixing$

$\Delta H_m = Enthalpy\ of\ mixing$

$\Delta S_m = Entropy\ of\ mixing$

$T = Absolute\ temperature$

The value of $T\Delta S_m$ is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$$\Delta H_m < T\Delta S_m \quad (2)$$

Figure 1 shows that the free energy involved in mixing is always negative or less than zero for the temperatures studied. The free energy decreases with increase in temperature as evident from Eq. 1. The results indicated that the blend will absolutely lead to a homogeneous mixture for the temperature range studied (50 to 500 K). The trend shows a very good compatibility between polyacrylic acid and poly12aDglucose with negative value of mixing energy, which may lead to form a perfect blend with significantly less effort.

Chi Parameter

The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similar components may lead to a high positive value of χ (chi).Figure 2 shows that the χ value is very small or negative for the temperature range studied (50 to 500 K) indicating very good mixing. The χ value increased with an increase in temperature upto 250 K and the value decreased with further increase in temperature. There is a very good possibility of homogeneous mixing with such small value of χ which agrees with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size. In this study the coordination number was found to be 6.46 +/- 0.04.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 3 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -1.9 kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 4 shows that the mixing energy for the system was small for the temperature range studied. The graph indicated that an increase in temperature increased the mixing energy. It also shows that mixing energy will be negative up to around 120 K, and the value gradually increases up to 0.6Kcal/Mol at a temperature of 270 K. However the mixing energy again reduces beyond the temperature 270 K. So, it is very much possible to mix the two components at any feasible temperature with least mixing energy value.The formation of nonhomogeneous blend with polyacrylic acid as base might help formation of blend with higher porosity such as hydrogel. This might have an application as adsorbent.

CONCLUSIONS

The possibility of use of polyacrylic acid and poly12aDglucose to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair can have very good compatibility at different ranges of temperature. The coordination number was found to be 6.46 +/- 0.04. The maximum number of configurations with respect to energy level was found to be -1.9 kcal/mol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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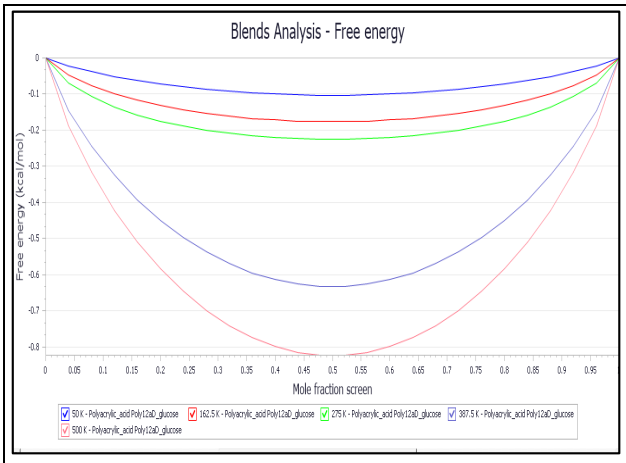

Figure 1. Free energy change with mole fraction of poly12aDglucose at different temperatures

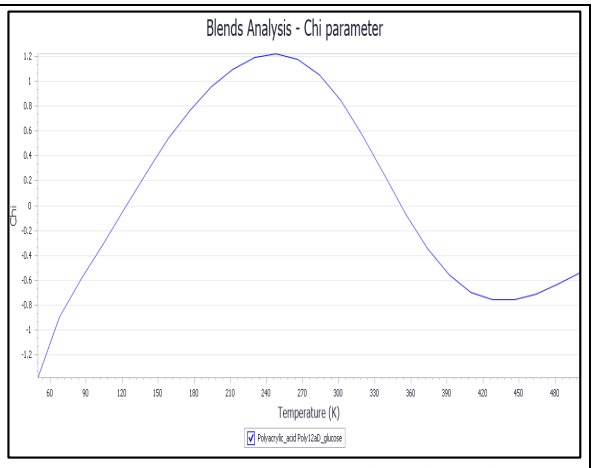

Figure 2. Change in χ (chi) value with temperature

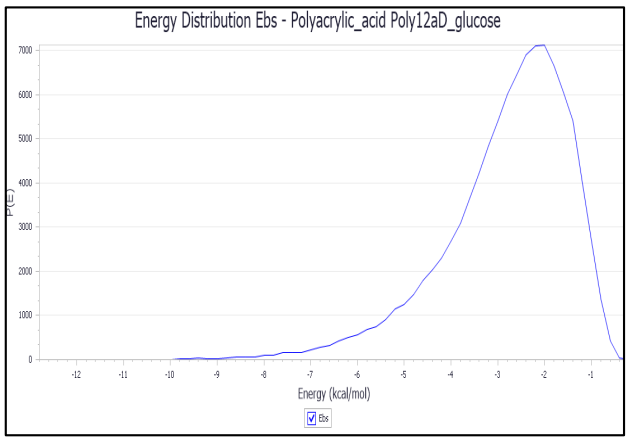

Figure 3. Energy distribution

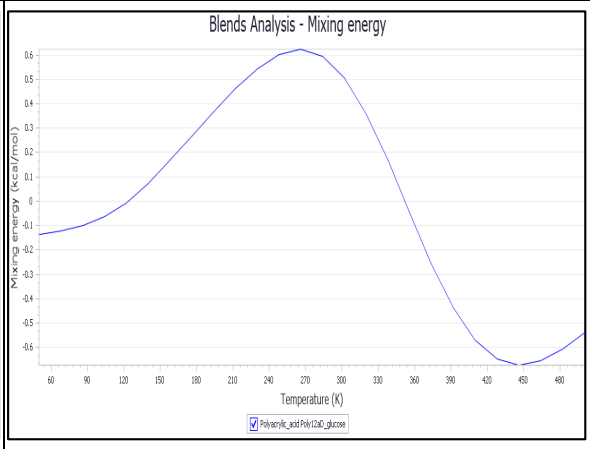

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyacrylic Acid and Polyacrylochloride Compatibility in a Blend

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ABSTRACT

A blend may be a mixture of more than one component. The specified property of a mix is its homogeneity. The choice of polyacrylic acid and polyacrylochloride to make a miscible blend was explored using Bio via Materials Studio. The compatibility of the 2 components was studied supported free energy of blending, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible only at heat. Phase diagram indicated that one phase are often obtained above 750 K which was the critical temperature. The coordination number was found to be 5.59 0.04. The very best number of configurations with reference to energy state was found to be -1.6 kcal/mol. The phase separation might cause its use as porous material to be used as adsorbent. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: blend, Bio via Materials Studio, polyacrylochloride, homogeneity

INTRODUCTION

Blends or composites are materials containing quite one component. The components don't lose their identity within the mixture. They combine and contribute to the property of the blend thereby improving the standard of the fabric. Development of one material with the specified property involves significant research and time. a mix utilizes the benefits of various materials, mix them to urge the specified property. Thus, a mix saves time to develop a replacement material thereby reducing the value of development of products with desired properties. Polymer blends are often made from two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the thanks to multi-functional materials. Polymers including carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] are reported to reinforce mechanical properties and water resistance. Researchers are performing on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; which will enhance flame retardancy without increasing the load [4]. Researchers have emphasized on synthesis and production of

lightweight composite materials having high strength important for enhancing fuel efficiency within the field of transportation [5]. There are applications of composites in structural Engineering thanks to high strength to weight ratio and resistance to corrosion. Thus, optical fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above-mentioned examples relied on laboratory experiments.Usually blends are prepared by trial and error method. Thus, it involves wastage of materials, time and money. Thus, researchers have focused on the utilization of in silico approach to develop new blends. Software (Materials Studio [7]) are wont to identify compatible pairs. Acrylic polymers have a good sort of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects etc. [8], bone repair [9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc. [10]. Polyacrylic acid may be a polyelectrolyte soluble in aqueous media at neutral pH it's used for preparing hydrogels. it's not toxic and doesn't cause irritation [11]. Researchers have used polyacrylochloride together with other materials to act as adsorbent [12]. Polyacrylochloride are reported to be utilized in Curtius reaction. This study is meant to spot the interaction of polyacrylic acid and polyacrylochloride to make blend.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systems of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

Polyacrylic acid and polyacrylochloride were prepared using the build menu of Materials Studio. The structure of the components was optimized using the components were used in blends->calculation menu of Materials studio. Polyacrylic acid was used as the base and polyacrylochloride was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acid and polyacrylochloride as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where $\Delta G_m = Gibb's free energy of mixing$

$\Delta H_m = Enthalpy of mixing$

$\Delta S_m = Entropy of mixing$

$T = Absolute temperature$

The value of $T\Delta S_m$ is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$\Delta H_m < T\Delta S_m$ (2)

Figure 1 shows that the free energy involved in mixing is always positive for the temperatures studied. The free energy decreases with increase in temperature as evident from Eq. 1. The results indicated that the blend will not lead to a homogeneous mixture for the temperature range studied (50 to 500 K). The trend suggested that there might be a possibility of a miscible blend at very high temperature.

Chi Parameter: The Flory–Huggins χ parameter describes the surplus free energy of blending and helps to elucidate phase behavior for polymer blends and block copolymers. For polymers which aren't chemically similar, a big mismatch in cohesive energy density results in a high χ value and, hence, a greater drive for phase separation. Thus, a high value of χ for chemically dissimilar polymers indicates poor mixing. For chemically similar polymers having small cohesive energy difference χ value is predicted to be small. However, there's an opportunity of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them during a mixture from occupying an equivalent configuration experienced within the pure phase. Polymer theory can predict that a mismatch in chain stiffness for chemically similar components may cause a high positive value of χ (chi).Figure 2 shows that the χ value is high for the temperature range studied (50 to 500 K) indicating demixing. The χ value decreased with increase in temperature. Thus, at heat there's an opportunity to make a miscible blend. The result's in agreement with the free energy of blending for the blend.

Coordination Number : The coordination number Zij is that the number of molecules of type j which will be packed around one molecule of type I. The coordination number was calculated for every of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It assumed that molecules aren't arranged on a daily lattice needless to say within the original Flory-Huggins theory. The coordination number is critical only the components of the binary blend have similar volumes or surface areas. it's difficult to use the pairs method in defining a coordination number for a binary numeration system during which the components aren't similar in size. During this study the coordination number was found to be 5.59 0.04.

Phase Diagram_: The compatibility of binary mixtures is often visualized by phase diagrams. Figure 3 shows the phase diagram for the 2 components of the blend. There are three regions of various degree of miscibility:

a. The single-phase miscible region existed above the critical temperature of around 750 K. This value supported the very fact that one phase blend is often formed at a heat (higher than 750 K).
b. Fragmented metastable regions existed between binodal and spinodal, and
c. The two-phase separated regions of immiscibility are bordered by the spinodal.

The binodal separated miscible (one-phase) and metastable region, while the spinodal separated the metastable and two-phase region.When the system enters from single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e., slow nucleation followed by growth of the phase separated domains. On the opposite hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distribution for Blend : The generation of various orientations using the pairs method may cause configurations of varying energy levels. Figure 4 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there's an extended, low-energy tail. The number of configurations with energy above the height value decreased significantly. The utmost frequency was observed for the energy state of around -1.6 kcal/mol.

Mixing Energy: A little value of blending energy can favor the blending process. Thus, the temperature at which the blending energy is low is often chosen for mixing. Figure 5 shows that the blending energy for the system was high for the temperature range studied. The graph indicated that a rise in temperature helped reduce the blending energy. This result supported the previous observations.The formation of nonhomogeneous blend with polyacrylic acid as base might help formation of blend with higher porosity such as hydrogel. This might have an application as adsorbent.

CONCLUSIONS

The possibility of use of polyacrylic acid and polyacrylochloride to make a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed supported free energy of blending, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible at heat. Phase diagram indicated that one phase is often obtained above 750 K. The coordination number was found to be 5.59 0.04. the utmost number of configurations with reference to energy state was found to be -1.6 kcal/mol. The phase separation might make it a porous material to be used as an adsorbent. Usually components for a mix are identified experimentally. This in silico study will help determine components of a mix without performing laboratory experiments saving materials, money and time.

ACKNOWLEDGMENTS

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12. Chromatographic Separation of As(DI), Sb(III) and Bi(HI) with Poly Calix-crown Hydroxamic Acid.

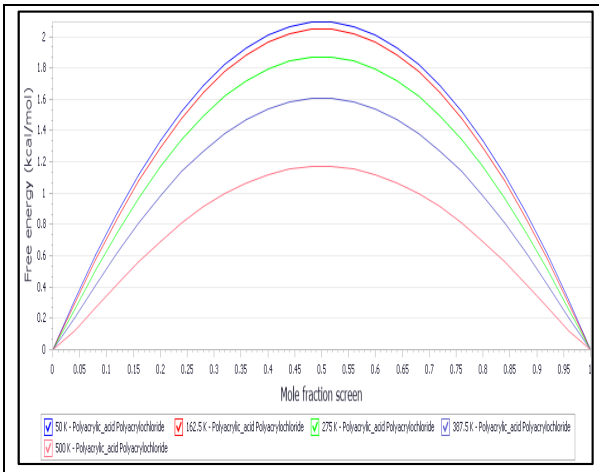

Figure 1. Free energy change with mole fraction of polyacrylochloride at different temperatures

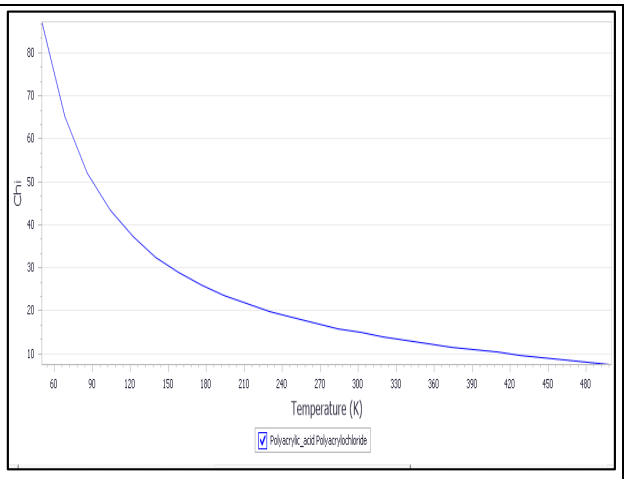

Figure 2. Change in χ (chi) value with temperature

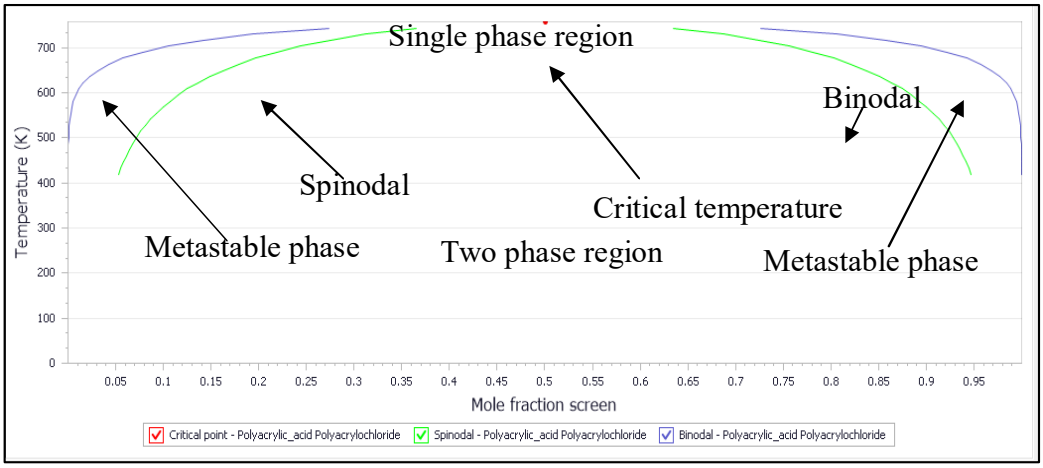

Figure 3. Phase diagram

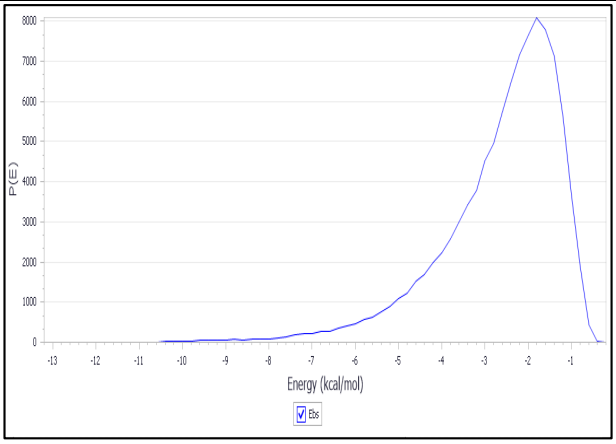

Figure 4. Energy distribution

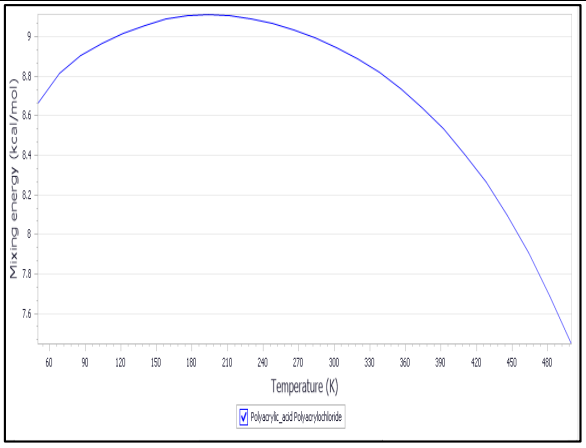

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyacrylic Acid and Polyacrylonitrile Compatibility in a Blend

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ABSTRACT

Chemical blending and chemical mixing are chemical processes which create a new chemical by combining two or more different raw materials. During mixing chemicals it is always desired to get a homogenous new material. The selection of polyacrylic acid and polyacrylonitrile to form a miscible blend was explored using Biovia Materials Studio. The compatibility of the two components was studied based on free energy of mixing, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible only at high temperature. Phase diagram indicated that a single phase can be obtained above 1000 K which was the critical temperature. The coordination number was found to be 5.38 +/- 0.04. The highest number of configurations with respect to energy level was found to be -1.8 kcal/mol. The phase separation might lead to its use as porous material to be used as adsorbent. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Chemical blending , Biovia Materials Studio, polyacrylonitrile

INTRODUCTION

Blends or composites are materials containing more than one components. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working

on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.Acrylic polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects etc. [8], bone repair [9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc. [10]. Polyacrylic acid is a polyelectrolyte soluble in aqueous media at neutral pH. It is used for preparing hydrogels. It is not toxic and does not cause irritation [11]. Researchers have found that poly acrylonitrile is thermoplastic and it does not melt under normal conditions, since it degrades before melting at above 300 °C [12]. Polyacrylonitrile also possesses a plasticizing effect on acrylic polymer and blocks the polar interactions between nitrile groups, and causes a lowering of melting point [13]. This study is intended to identify the interaction of polyacrylic acid and polyacrylonitrile to form blends.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

Polyacrylic acid and Poly acrylonitrile were prepared using the build menu of Materials Studio. The structure of the components were optimized using the components used in blends->calculation menu of Materials studio. Polyacrylic acid was used as the base and Poly acrylonitrile was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acid and Poly acrylonitrile as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where ΔG_m = *Gibb's free energy of mixing*

ΔH_m = *Enthalpy of mixing*

ΔS_m = *Entropy of mixing*

T = *Absolute temperature*

The value of $T\Delta S_m$ is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$$\Delta H_m < T\Delta S_m \quad (2)$$

Figure 1 shows that the free energy involved in mixing is always positive with very small values for the temperatures studied. The free energy decreases with increase in temperature as evident from Eq. 1. The results indicated that the blend will not lead to a homogeneous mixture for the temperature range studied (50 to 500 K). However the graph indicated that a slight increase in temperature above 500 K might help formation of a homogeneous mixture.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similar components may lead to a high positive value of χ (chi).Figure 2 shows that the χ value is high for the temperature range studied (50 to 500 K, excluding 210-260 K) indicating demixing. The χ value was significantly small at the temperature 210 to 260 K , enhancing a possibility of forming a somewhat miscible blend at this temperature.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size. In this study the coordination number was found to be 5.38 +/- 0.04.

Phase Diagram: The compatibility of binary mixtures can be visualized by phase diagrams. Figure 3 shows the phase diagram for the two components of the blend. There are three regions of different degree of miscibility:

a. The single-phase miscible region existed above the critical temperature of around 800 K and also at a temperature between 200 K to 300 K with a very less value of mole fraction (0 to 0.07) and also at a very high mole fraction value of polyacrylonitrile beyond 0.94. This value supported the fact that single phase blend can be formed at different temperatures with specific mole fraction value.
b. Fragmented metastable regions existed between binodals and spinodals, and
c. The two-phase separated regions of immiscibility are bordered by the spinodals.

The binodals separated miscible (one-phase) and metastable region, while the spinodals separated the metastable and two-phase region.When the system enters from single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e, slow nucleation followed by growth of the phase separated domains. On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 4 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat a symmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -1.6 kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 5 shows that the mixing energy for the system was high for the temperature range studied. The graph indicated that an increase in temperature increased the mixing energy. The formation of nonhomogeneous blend with polyacrylic acid as base might help formation of blend with higher porosity such as hydrogel. This might have an application as adsorbent/absorbent.

CONCLUSIONS

The possibility of use of polyacrylic acid and polyacrylonitrile to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible at high temperature. Phase diagram indicated that a single phase can be obtained above 750 K as well as around 200 K depending on the mole fraction. The coordination number was found to be 5.59 +/- 0.04. The maximum number of configurations with respect to energy level was found to be -1.6 kcal/mol. The phase separation might make it a porous material to be used as an adsorbent. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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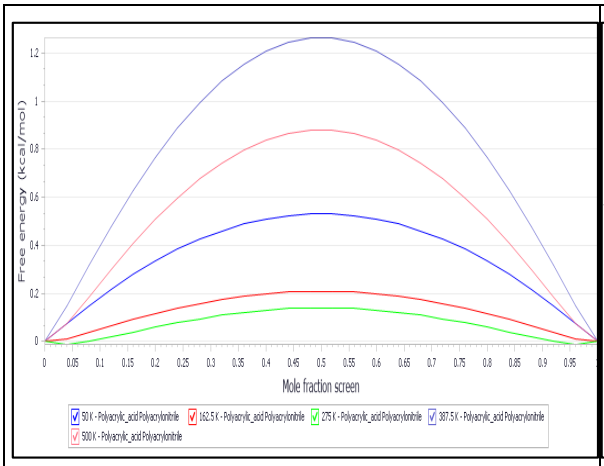

Figure 1. Free energy change with mole fraction of polyacrylonitrile at different temperatures

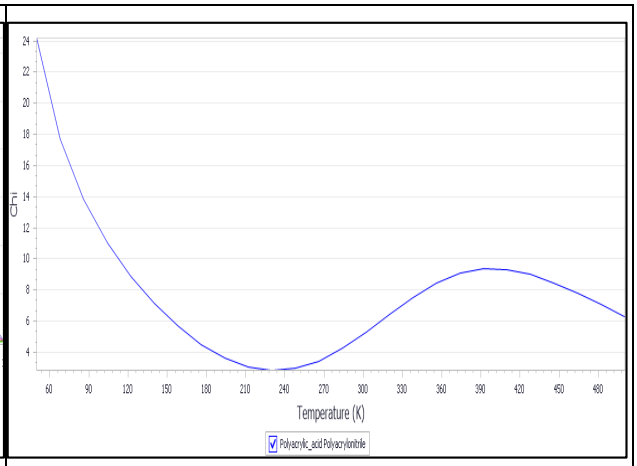

Figure 2. Change in χ (chi) value with temperature

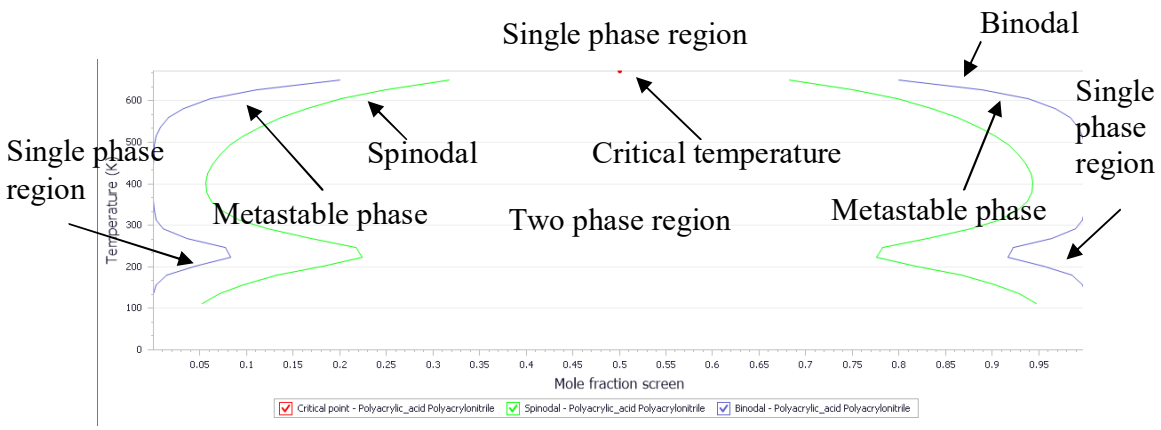

Figure 3. Phase diagram

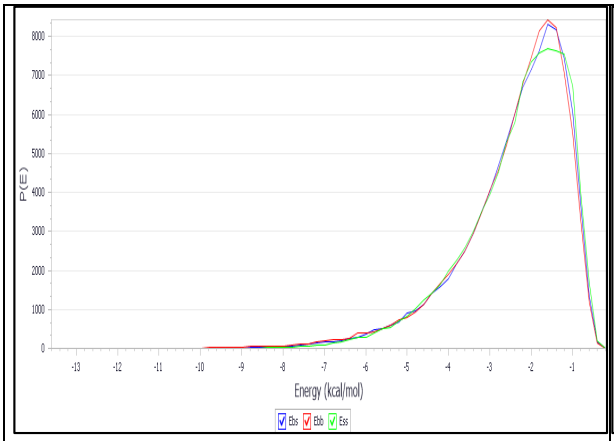

Figure 4. Energy distribution

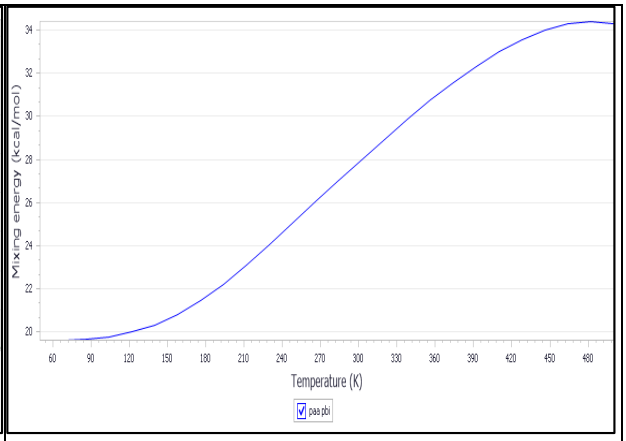

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyacrylic Acid and Polymethylacrylate Compatibility in a Blend

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ABSTRACT

A blend can be defined as the mixture of more than one components and it is desired to have homogeneity in a blend. The selection of polyacrylic acid and polymethylacrylate to form a miscible blend was explored using Biovia Materials Studio. The compatibility of the two components was studied based on free energy of mixing, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible only at high temperature. Phase diagram indicated that a single phase can be obtained above 750 K which was the critical temperature. The coordination number was found to be 5.24 +/- 0.04. The highest number of configurations with respect to energy level was found to be -2.4 kcal/mol. The phase separation might lead to its use as porous material to be used as adsorbent. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: blend, polymethylacrylat, chi parameter, porous material

INTRODUCTION

Blends or composites are materials containing more than one components. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.

Acrylic polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects etc. [8], bone repair [9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc. [10]. Polyacrylic acid is a polyelectrolyte soluble in aqueous media at neutral pH It is used for preparing hydrogels. It is not toxic and does not cause irritation [11]. Researchers have used polymethylacrylate in combination with other materials such as SiO_2 to increase the thermal stability [12]. Polymethylacrylate has been reported to be used as solid state fluorescent material [13].This study is intended to identify the interaction of polyacrylic acid and polymethylacrylate to form blends.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

Polyacrylic acid and polymethylacrylate were prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyacrylic acid was used as the base and polymethyl acrylate was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acid and polymethylacrylate as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where ΔG_m = Gibb's free energy of mixing

ΔH_m = Enthalpy of mixing

ΔS_m = *Entropy of mixing*

T = *Absolute temperature*

The value of $T\Delta S_m$ is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$$\Delta H_m < T\Delta S_m \quad (2)$$

Figure 1 shows that the free energy involved in mixing is always positive for the temperatures studied. The free energy decreases with increase in temperature as evident from Eq. 1. The results indicated that the blend will not lead to a homogeneous mixture for the temperature range studied (50 to 500 K). The trend suggested that there might be a possibility of a miscible blend at very high temperature.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similar components may lead to a high positive value of χ (chi).Figure 2 shows that the χ value is high for the temperature range studied (50 to 500 K) indicating demixing. The χ value decreased with increase in temperature. Thus at high temperature there is a possibility to form a miscible blend. The result is in agreement with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size. In this study the coordination number was found to be 5.24 +/- 0.04.

Phase Diagram: The compatibility of binary mixtures can be visualized by phase diagrams. Figure 3 shows the phase diagram for the two components of the blend. There are three regions of different degree of miscibility:

a. The single-phase miscible region existed above the critical temperature of around 2200 K. This value supported the fact that a single phase blend can be formed at a high temperature (higher than 2200 K).
b. Fragmented metastable regions existed between binodals and spinodals, and
c. The two-phase separated regions of immiscibility are bordered by the spinodals.

The binodals separated miscible (one-phase) and metastable region, while the spinodals separated the metastable and two-phase region.When the system enters from single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e, slow nucleation followed by growth of the phase separated domains. On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 4 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -2.4 kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 5 shows that the mixing energy for the system was high for the temperature range studied. The graph indicated that an increase in temperature increased the mixing energy. Figure 5 shows that mixing energy will be less up to around 300K. Thus, it is possible to mix the two components at this temperature. However, the phase diagram suggests that there will be phase separation.The formation of nonhomogeneous blend with polyacrylic acid as base might help formation of blend with higher porosity such as hydrogel. This might have an application as adsorbent.

CONCLUSIONS

The possibility of use of polyacrylic acid and polymethyl acrylate to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible at high temperature. Phase diagram indicated that a single phase can be obtained above 2200 K. The coordination number was found to be 5.24 +/- 0.04. The maximum number of configurations with respect to energy level was found to be -2.4 kcal/mol. The phase separation might make it a porous material to be used as an adsorbent. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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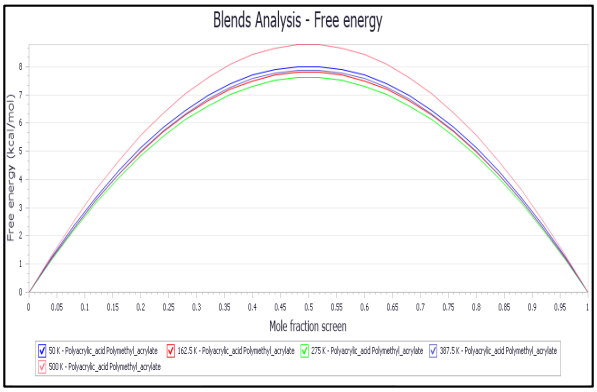

Figure 1. Free energy change with mole fraction of polymethyl acrylate at different temperatures

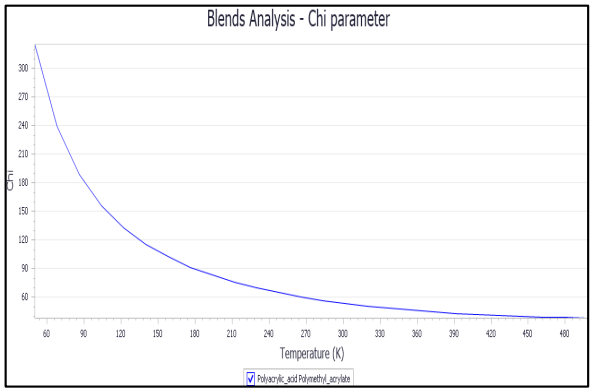

Figure 2. Change in χ (chi) value with temperature

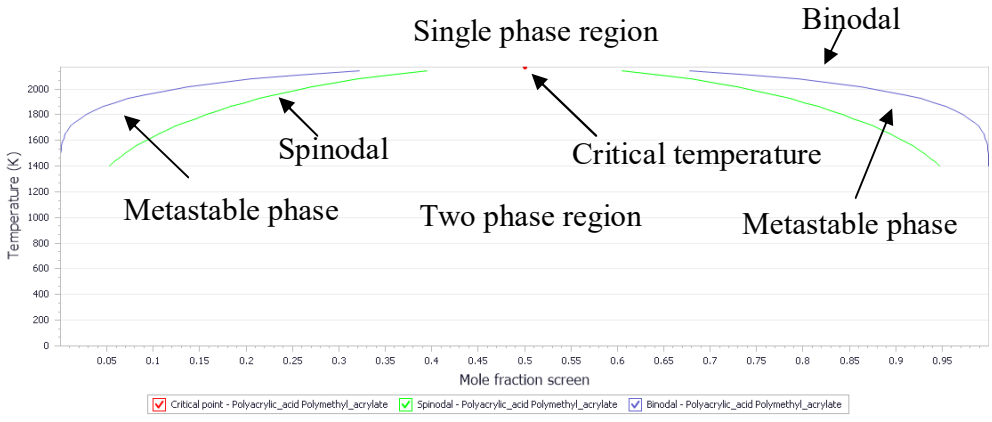

Figure 3. Phase diagram

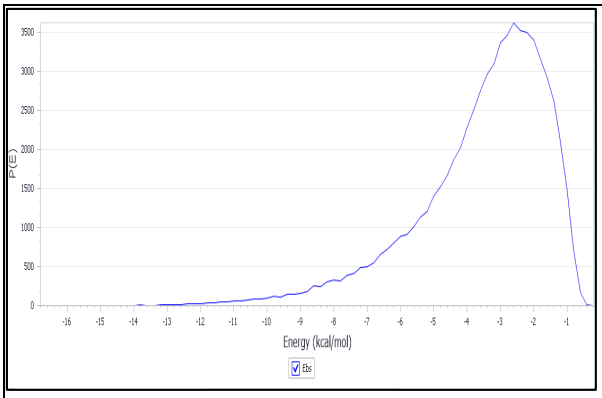

Figure 4. Energy distribution

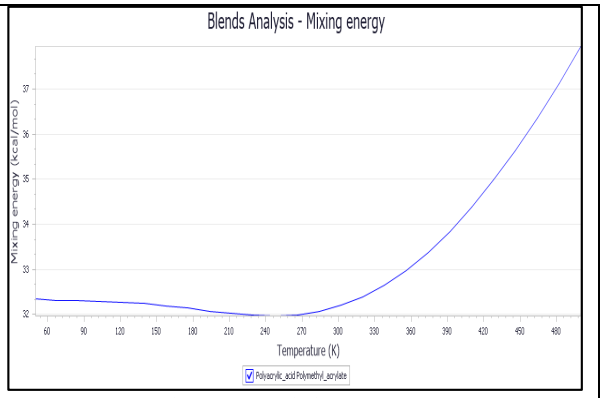

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyvinyl Alcohol and Polyvinyl Chloride Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of polyvinyl alcohol and polyvinylchloride to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The mechanical properties of the compositewere studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of vinyl alcohol.This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: In silico analysis, blend, mechanical property, Biovia Materials Studio, polyvinyl alcohol.

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi-functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of

transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus; researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Polymerization of monomers containing vinyl group leads to the formation of vinyl polymers such as polyvinyl chloride [8], poly styrene [9], polyvinyl esters [10], polyvinyl acetate [11, 12] etc.

Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [13, 14]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [15]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [16].

Polyvinyl Chloride (PVC or Vinyl) is a high strength thermoplastic material having wide applications in the manufacture of pipes, medical devices, wire and cable insulation the list is endless. It is the world's third-most widely produced synthetic plastic polymer for its superior mechanical and physical properties. However, the fluid plasticity and thermal stability of PVC are inferior to those of other commodity plastics such as polyethylene and polystyrene [17]. Much work on improvement of the inferior properties of PVC has been carried out besides the addition of additives such as plasticizers, heat stabilizers, lubricants, fillers and other polymers [18]. This study is intended to identify the interaction of polyvinyl alcohol and polyvinyl chloride to form blends.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

The structures of polyvinyl alcohol and polyvinyl chloride were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS & DISCUSSION

In this work the use of polyvinyl alcohol and polyvinyl chloride as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group contribution methods are being used for several years to estimate the properties of polymers and other small molecules. These techniques have the advantages of quick calculation, user friendly approach and do not need any specialized

knowledge.As a result of this, these methods are well accepted and vastly used to predict the properties of range of molecules and polymers. However, the fundamental limitation of this group contribution method lies over the fact that it needs a strong set of database of group contribution based on which it could predict the desired properties.Therefore, if a polymer contains certain groups whose group contribution values have not been assigned, then it is difficult to predict the property of that polymer.

Synthia adopt a different approach to overcome the group contribution limitation wherein topological information was utilized to predict the properties.The connectivity indices derived from graph theory are employedand the database of group contribution is not necessary to predict the properties. Therefore, the polymer properties could be estimated for any kind of polymer that composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Bulk modulus: Bulk modulus is the measure of the decrease in volume with an increase in pressure. As can be seen from Figure 1, there is a rise in the bulk modulus of the composite upon increasing the mass fraction of the vinyl alcohol.

Shear modulus: It is one of the ways in measuring the stiffness of the polymer composite. It shows the responseof the composite to shear deformation. As depicted in Figure 2, upon increasing the mass fraction of vinyl alcohol, the shear modulus of the composite increases linearly.

Young's modulus: In the linear elasticity region, young's modulus is the ratio of stress and strain. It compares the relative stiffness of the composite. Figure 3 shows that upon increasing the mass fraction of vinyl alcohol, the Young's modulus of the composite increases linearly.

Poisson ratio: It is defined as the ratio of transverse strain to axial strain. As illustrated in Figure 4, Poisson ratio of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Brittle fracture stress: This is an unstable process where fracture in the material takes place even before any plastic degradation. Figure 5 shows that the brittle fracture stress of the composite increases linearly with increase in mass fraction of vinyl alcohol.

CONCLUSION

The possibility of use of polyvinyl alcohol and polyvinyl chloride to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to mechanical properties.The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of vinyl alcohol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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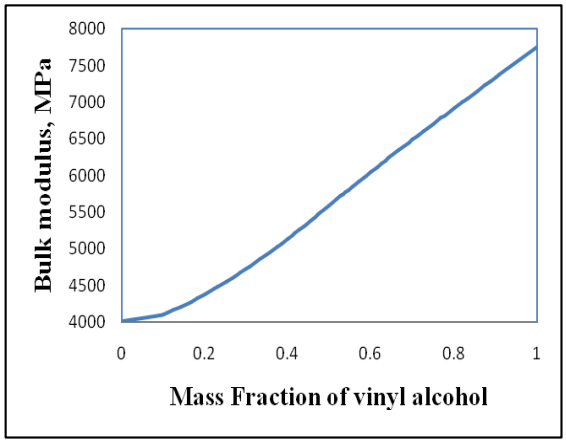

Figure 1. Change in bulk modulus with mass fraction of vinyl alcohol

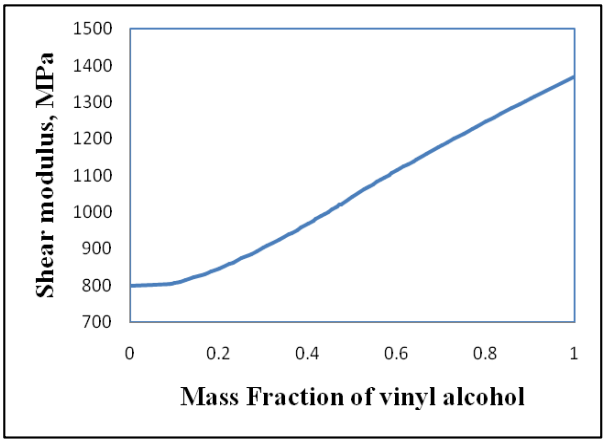

Figure 2. Change in shear modulus with mass fraction of vinyl alcohol

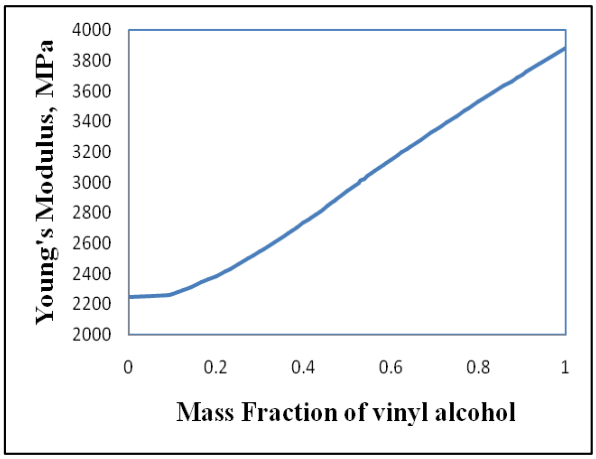

Figure 3. Change in Young's modulus with mass fraction of vinyl alcohol

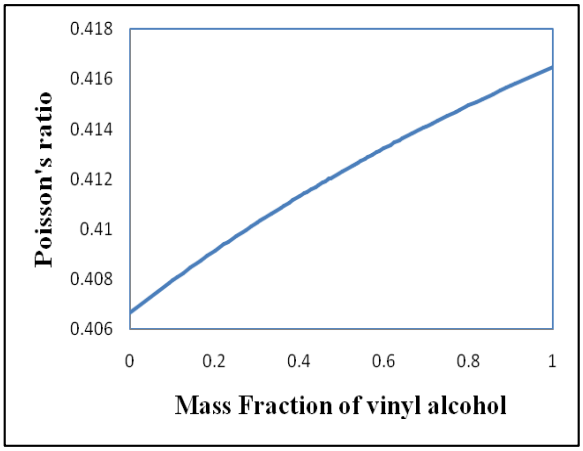

Figure 4. Change in Poisson modulus with mass fraction of vinyl alcohol

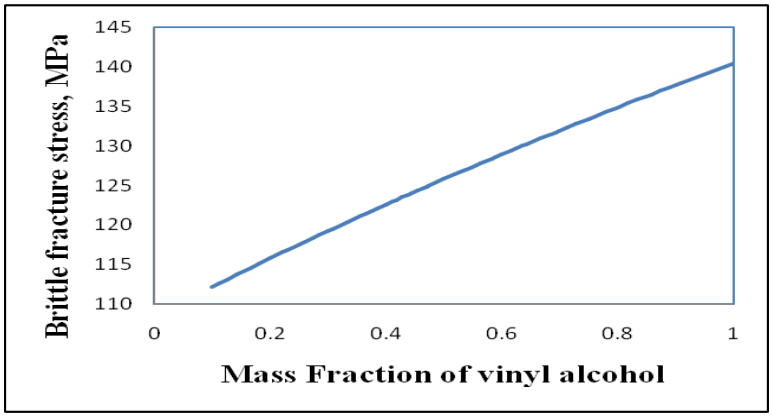

Figure 5. Change in brittle fracture stress with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyvinyl Alcohol and Poly-1,2-α-D-glucose

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ABSTRACT

This article provides the theoretical information of a blendof two monomers with varying mass fraction concerning their gas permeability properties. Blend is a mixture of more than one component. The desired property of a blend is its homogeneity, perhaps it may be heterogeneous.Vinyl alcohol and 1,2-α-D-glucosemonomers are considered to be the indivisual components to get the desired mechanical properties of the blend. This study is explored using Biovia Materials Studio synthia analysis. The permeability properties of the polymer composite were analyzed concerning with varying mass fraction of components. The molar volume and density decreased with an increase in vinyl alcoholmass fraction. The permeability properties of the composite were studied based on the permeability of oxygen, nitrogen, and carbon dioxide. The results showed that the permeability of all the gases decreased with the increase in the mass fraction of vinyl alcohol. This study will help to determine pairs without performing laboratory experiments, saving materials, money, and time.

Keywords: Synthia, in silico, polyvinyl alcohol, poly-1, 2-α-D-glucose, biovia material studio, gas permeability

INTRODUCTION

Blends or composites are the physical combination of more than one component where components do retain their identity in the mixture. The blend may be a homogenous or heterogeneous mixture. A single material cannot provide multiple anticipated properties. It is desirable to combine different components thereby improving the properties of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus blending is a process which provides an easy pathway develop a new material by reducing the cost of development of products with

preferred properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.A composite/blend possess significantly different chemical andphysical characteristics from those of its constituent components. In a composite the constituents remain physically separable and distinct from each other. Usually, a composite is a matrix in which strong and stiff reinforcement is distributed but made of a soft and weaker component [1-3].The upgraded properties of composites are predominantly governed by their microstructure and interaction between matrix and reinforcing materials in the inter-phase region [4, 5].Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [6] have drawn significant attention in recent years. Biodegradable polymers- natural fiber composites [7] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [8]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [9].

Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [10]. There are applications of composites in structural engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [11] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method and this technique is a low cost and less time consuming method. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [12]) has been used to identify compatible pairs. Polyvinyl alcohol (PVA) is a promising material among several polymers that have high dielectric strength, easy film formation, and adhesiveness. These properties can be modified by dopant concentrations [13, 14]. Moreover, due to their high mechanical strength, environmental stability, easy processability, and film forming ability, PVA is usually used in packaging industry to form strong polymeric films [15]. In addition, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [16].

Researchers have found applications of glycopolymers (synthetic polymers containing pendant carbohydrate groups) in the separation and removal of toxins and bacteria, tumor cell recognition and glucose-responsive insulin delivery [17]. It has been found that biopolymer blends possess good thermal stability [18].By adding glycopolymers (cellulose nanoscale fillers) in different polymers (polyvinyl alcohol or polylactic acid) we can generate nanocomposites resulting in mechanical reinforcement and alternation of other properties [19].This study is intended to identify the interaction of polyvinyl alcohol and poly-1, 2-α-D-glucose to form blends.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systems of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

The structures of polyvinyl alcohol and poly-1, 2-α-D-glucose were fed to the synthia menu of Materials Studio. It was then run for different mass fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of mass fraction of polyvinyl alcohol on the mechanical properties of the composite. The structures of poly vinyl alcohol and Poly Ethyl Urethane were fed to the

synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of poly vinyl alcoholon the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work, the use of polyvinyl alcohol and poly-1, 2-α-D-glucose as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties.From several years, group additive methods are used to estimate the properties of polymers and other molecules. These methods are quick and can be used easily that eventually leads to wide utilization to estimate the properties of materials. Moreover, these techniques do not require any specific expertise and the values from database are extracted that each group could contribute for a specific property. Finally, the values for each group are added that makes up the material/composite. However, the primary limitation that exist with these methods lies with the fact that, the property of a material may not be determined if the group contribution value is not available for a particular group that makes up the molecule.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite decreases with an increase in the mass fraction of vinyl alcohol.

Density: Decrease in density indicates increase in the porosity. A higher porosity will enhance the surface area making it suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite decreases linearly with increase in the mass fraction of vinyl alcohol.

Permeability of gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium.Lower permeability indicates a longer time lag for the gas to pass through the membrane. Figure 3 show that the permeability of oxygenthrough the composite decreases with increase in the mass fraction of vinyl alcohol.

Figure 4 show that the permeability of nitrogenthrough the composite decreases with increase in mass fraction of vinyl alcohol. Figure 5 show that the permeability of carbon dioxidethrough the composite decreases with increase in mass fraction of vinyl alcohol. Thus the results indicated that an increase in vinyl alcohol fraction reduces the permeability of different gases. The rate of permeability might be influenced by the molecular weight of the gases. The decrease in the permeability of the gases makes the composite suitable for the development of packaging materials.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly-1,2-α-D-glucose to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties of different gases like Oxygen, Nitrogen, and carbon dioxide.The molar volume and density decreased with an increase in vinyl alcohol fraction. The permeability properties of the composite were studied based on the permeability of

oxygen, nitrogen, and carbon dioxide. The results indicated that the permeabilityof all the gases decreased with the increase in the mass fraction of vinyl alcohol. Usually, components of a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments, saving materials, money, and time.

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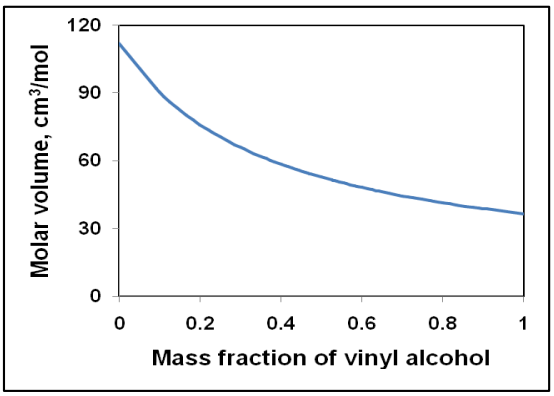

Figure 1. Change in molar volume with the mass fraction of vinyl alcohol.

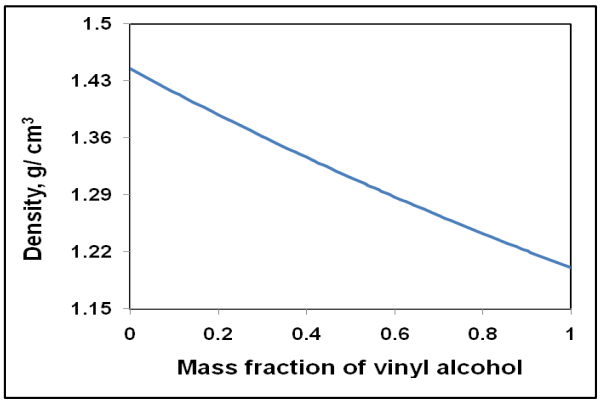

Figure 2. Change in density with the mass fraction of vinyl alcohol

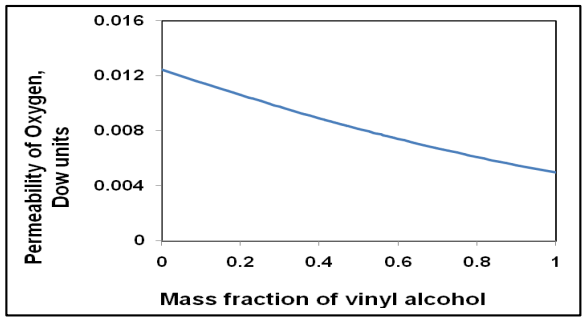

Figure 3. Change in permeability of oxygen with mass fraction of vinyl alcohol

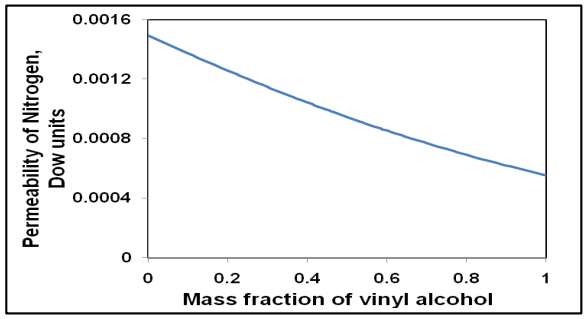

Figure 4. Change in permeability of nitrogen with mass fraction of vinyl alcohol

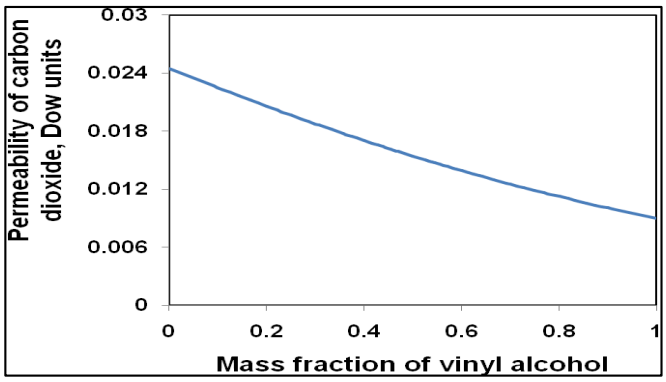

Figure 5. Change in permeability of carbon dioxide with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyvinyl Alcohol and Polyvinyl Chloride Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of polyvinyl lalcohol and polyvinylchloride to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in vinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases decreased with increase in mass fraction of vinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: In silico analysis, gas permeability, polyvinyl alcohol, blend, Biovia Materials Studio.

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi-functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of

lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money.Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Polymerization of monomers containing vinyl group leads to the formation of vinyl polymers such as polyvinyl chloride [8], poly styrene [9], polyvinyl esters[10], polyvinyl acetate[11, 12] etc.

Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [13, 14]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [15]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [16].

Polyvinyl Chloride (PVC or Vinyl) is a high strength thermoplastic material having wide applications in the manufacture of pipes, medical devices, wire and cable insulation...the list is endless. It is the world's third-most widely produced synthetic plastic polymer for its superior mechanical and physical properties. However the fluid plasticity and thermal stability of PVC areinferior to those of other commodity plastics such as polyethylene and polystyrene [17]. Much work on improvement of the inferior properties of PVC has been carried out besides the addition of additives such as plasticizers, heat stabilizers, lubricants, fillers and other polymers [18].This study is intended to identify the interaction of polyvinyl alcohol and polyvinyl chloride to form blends.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

The structures of polyvinylalcohol and polyvinyl chloride were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinylalcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and polyavinyl chloride as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. From several years, group additive methods are used to estimate the properties of polymers and small molecules as well. The wide application of these methods is due to their user-friendliness and fastness in calculations. Furthermore, these techniques do not require in depth knowledge of intermolecular interactions to predict the properties and it solely

depends upon the database containing the group contribution values. However, the primary limitation with these techniques lies with the fact that, for a new material/polymer that constitutes new groups, the group additive methods may not determine the properties as there will be no data for the new groups in the database. To overcome this limitation, topological information was utilized in Synthia to estimate the properties of polymers. The connectivity indices derived from the graph theory are employed to predict the properties rather than using the group contribution values from the database. Therefore, properties of the polymers that composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine can be determined using Synthia.

Molar volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Density: Increase in density indicates decrease in porosity. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Permeability of gas: Permeability determines the speed at which the gas can pass through the polymer membrane after it is accumulated in the higher potential side of the membrane.Lower permeability indicates longer time lag for the gas to pass through the membrane. Figure 3 shows that the permeability of oxygenthroughthe composite decreases with increase in mass fraction of vinyl alcohol.

Figure 4 show that the permeability of nitrogenthrough the composite decreases with increase in mass fraction of vinyl alcohol. Figure 5 show that the permeability of carbon dioxidethrough the composite decreases with increase in mass fraction of vinyl alcohol. Thus the results indicated that an increase in vinyl alcohol fraction reduces the permeability of different gases. The rate of permeability might be influence by the molecular weight of the gases.

CONCLUSION

The possibility of use of polyvinyl alcohol and polyvinyl chloride to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in vinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeability for all the gases decreased with increase in mass fraction of vinyl alcohol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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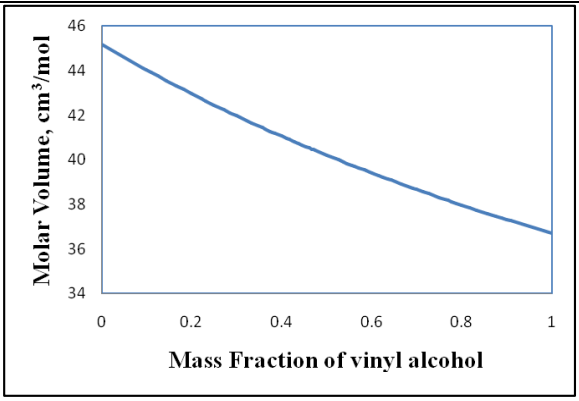

Figure 1. Change in molar volume with mass fraction of vinyl alcohol

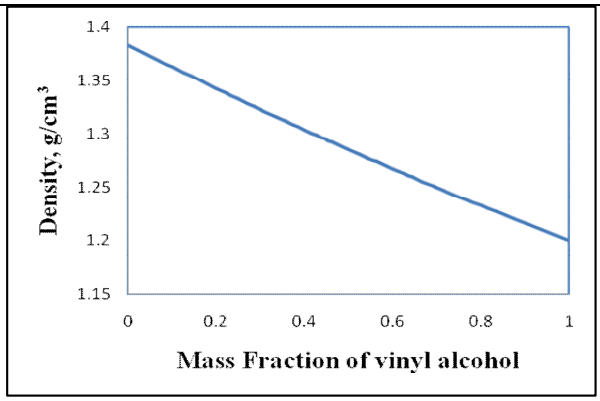

Figure 2. Change in density with mass fraction of vinyl alcohol

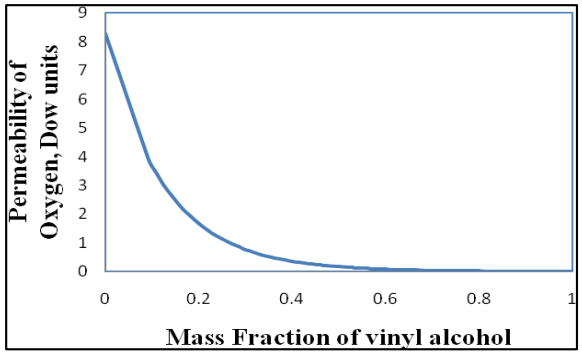

Figure 3. Change in permeability of oxygen with mass fraction of vinyl alcohol.

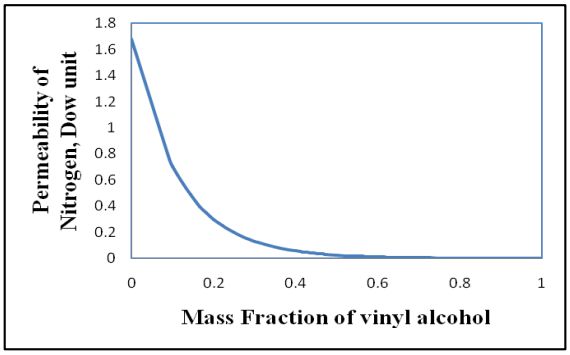

Figure 4. Change in permeability of nitrogen with mass fraction of vinyl alcohol

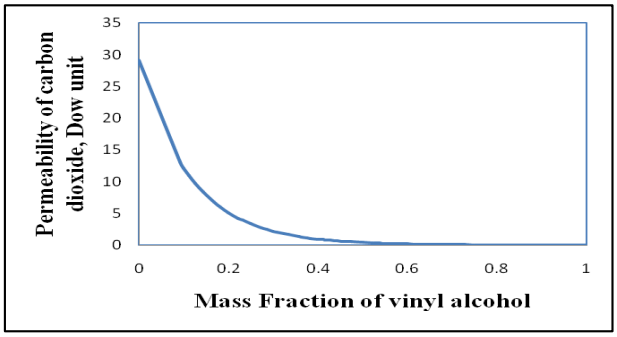

Figure 5. Change in permeability of carbon dioxide with mass fraction of vinyl alcohol.

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Poly (Biphenyl Dimethylcarbonate) and Polyether Sulfone (PES) Blend Membrane

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ABSTRACT

Hybrid polymers with improved gas barrier properties are the major concern of packaging application. As blends are the selective combination of two or more polymeric components to get the desired one with low cost, it can be more easily adopted for mass production. The optimum blend composition of poly (biphenyl dimethylcarbonate)and polyether sulfone (PES) to provide the desired gas barrier properties was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties towards various gases. The molar volume was found to be increased, while density was decreased with increase in the mass fraction of poly(biphenyl dimethylcarbonate) (PC). The permeability properties of the blend were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases increases with increase in mass fraction of poly (biphenyl dimethyl carbonate). This study will help determine pairs without performing laboratory experiments saving materials, money and time

Keywords: Gas permeability, Hybrid, In-silico analysis, Compatibility, Packaging

INTRODUCTION

Polymeric blends are usually offered improved physical and chemical properties like thermal, mechanical, gas barrier and biodegradability [1]. These properties are the prime interest for the researchers to design best packaging material. Gas permeability is sometimes offered as essential criterion to design the polymer for biomedical and industrial utilization. For instance, polymers with high barrier properties, i.e. low permeability, are mandatory for food packaging applications to prevent loss of aroma, color and food-value and to slow down spoilage [2]. Apart from this food packaging application; there are lots of other applications which require the polymers to have high, low or tailored permeability like, filters and membranes for gas or liquid separation [3], protective coatings (e.g., paints and varnishes) [4], polymer coatings for controlled drug release [5] and water desalination [6].The permeability of liquids and gases through polymer membranes (plastic films) may be happened by either a

temperature or pressure gradient, or by concentration gradient or external force field. The "solution-diffusion" mechanism is generally used to depict the pathway of gas permeation. It involvesthree steps. In the first step absorption of small molecules is happened into the membrane at the side of higher gradient (concentration, pressure, etc). On the other hand, second step involves the molecular diffusion through the membrane and the final step is related to desorption of those molecules from the membrane at the opposite side of lower gradient. The gas permeability in a polymer is generally varied with the nature of polymer and permeates. It may be accounted due to various degree of crystallinity and porosity of the polymers along with surface functionality (hydrophilic/ hydrophobic groups).The main aim of combining polymeric materials is to achieve the desired quality of the material. Among various polymers, polybiphenyldimethyl carbonate (PC) is a widely used engineering plastics because of its physical and chemical properties like ductility, good thermal stability, excellent transparency, and high mechanical strength[7]. As a resultof these excellent properties, PC has been largely employed in electronic and electronic appliances along with automotive industry, having an annual production of 6 million tons.

Recent report by Behboudi et. al. [8] shows thatPC is blended withpolyvinyl chloride (PVC)to preparethe ultrafiltration membrane for water purification. On the other hand, PC is also blended with poly(vinylidene fluoride) (PVDF) to prepare mechanically strong multicomponent nano composites with nano structural reinforcement of graphene nanoplates, carbon nanotube, and organically modified montmorillonite [9]. In another recent report Wen et al. reinforced the graphene plates into blend of polybutyleneterethalate and polycarbonate [10] to obtain electrical and thermal conductive materials. The unique material, formed from the blend of PC with polystyrene is also reported to sense organic vapours with incorporation of multiwalled carbon nanotubes (MWCNTs) [11]. Polycarbonate blended polysulfone material is recently observed to have improved thermal and mechanical properties [12]. Therefore, investigation of blending compatibility of polycarbonate with other polymer is the urgent need of current research to develop advanced functional materials. All the above mentioned examples relied on laboratory experiments. Usually, preparation of homogeneous blend in wet-lab condition, requires huge time and wastage of materials which can be minimized by in-silico approach through material studio [13] of "Biovia" software.. In present context, we are focusing to optimize the homogeneous blend composition of polybiphrnyldimethylcarbonate (PC) with polyether sulfone (PES) in terms of gas permeability. Among various engineering polymers, polyether sulfone (PES) is a high-temperature sustaining thermoplastic polymer with striking strength and chemical stability from various organic solvents. It belongs to the polysulfone family and contains an aryl-SO_2 subunit in their long chain structures. Nonetheless, the inherent hydrophobic property of PES makes this material sensitive to membrane fouling, restricting its more extensive applications in membrane based water treatment. Due to high chemical stability it is also preferably used for gas separation in harsh environment.

To improve the gas separation efficiency of PES, a few investigations have been performed. In a report, Adib et al. [14] incorporated the nanostructural silica to improve the gas separation. However, blending of PES with other hydrophilic polymer is one of the easiest routes to improve the efficiency of the gas separation. In another report, Mannan et al. [15] investigated the gas-permeation behavior of glassy poly(vinyl acetate) (PVAc)–PES hybrid films and PSF–PES film. Interestingly, it is found that the gas permeation properties of hybrid PSF–PES film is remain unaltered as compared to the properties of polyether sulfone. However on account of the PES–PVAc hybrid polymer, low selectivity was observed for gas separation and may be accounted as the phase separation in their blend. Kamal et al. [16] revealed that the blend with elastomers (like polydimethylsiloxane) leads to the improved gas permeation properties of the polydimethylsiloxane–PES hybrid. Akbarian et al.[17] prepared the PES based blend membranes for CO_2 gas separation with inclusion polyethylene glycol (PEG) as second polymer.Therefore, the present in-silico approach of blend analysis between poly(biphenyl dimethyl carbonate) (PC) and polyether sulfone (PES) may be utilized to optimize the composition to fabricate desirable functional materials with some improved physical and chemical properties.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

The structures of poly (biphenyl dimethylcarbonate) and polyether sulfone (PES) were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of Poly(biphenyl dimethylcarbonate) on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of poly(biphenyl dimethylcarbonate)and polyether sulfone as potential components of a blend was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the blend hybrid increasedlinearly with increase in mass fraction of biphenyl dimethyl carbonate.

Density: Decrease in density indicates the enhancement of porous morphology. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows the density variation of the blend which showed a linear decrease with increase in mass fraction of biphenyl dimethyl carbonate. This decrease in density along with increase of molar volume indicates the phase separation of individual polymeric components and therefore, creating porous morphology.

Permeability of Gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium.Lower permeability indicates longer time lag for the gas to pass through the membrane. Figure 3shows that the permeability of oxygenthrough the blend hybrid increasedwith increase in mass fraction of biphenyl dimethyl carbonate. On the other hand, Figure 4 shows that the permeability of nitrogenthrough the hybrid blend increasedwith increase in mass fraction of biphenyl dimethyl carbonate. In the same analogy and as expected, Figure 5shows that the permeability of carbon dioxidethrough the blend hybrid increased with increase in mass fraction of biphenyl dimethyl carbonate.

Thus the results indicated that an increase in biphenyl dimethyl carbonate fraction increased the permeability of different gases. The rate of permeability might be influence by the molecular weight of the gases.

CONCLUSION

The possibility of use of poly (biphenyl dimethylcarbonate) and polyethersulfoneto form aadvanced adsorbent material was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties.The molar volume increased, while density decreased with increase in biphenyl dimethyl carbonate fraction due to formation of porous morphology. The permeability properties of the blend hybrid were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeabilityfor all the gases increased with increase in mass fraction of biphenyl dimethyl carbonate. Usually components for a blend are identified experimentally. This in-silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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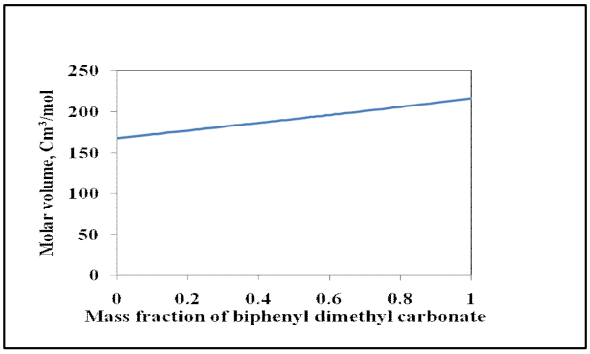

Figure 1. Change in molar volume with mass fraction of biphenyl dimethyl carbonate

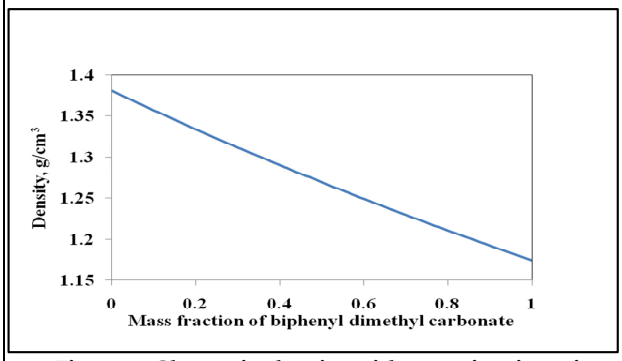

Figure 2. Change in density with mass fraction of biphenyl dimethyl carbonate

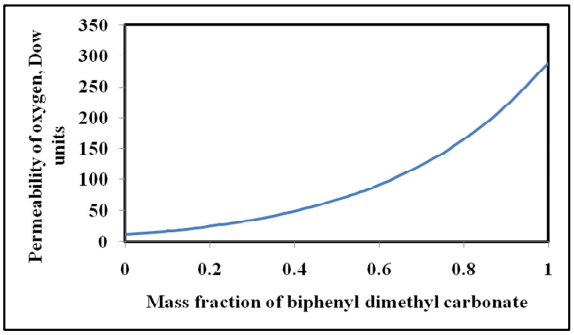

Figure 3. Change in permeability of oxygen with mass fraction of biphenyl dimethyl carbonate

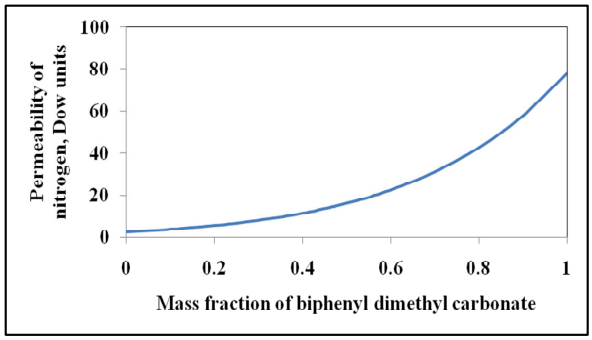

Figure 4. Change in permeability of nitrogen with mass fraction of biphenyl dimethyl carbonate

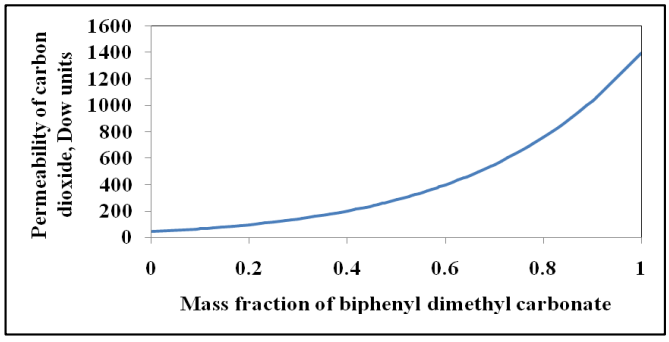

Figure 5. Change in permeability of carbon dioxide with mass fraction of biphenyl dimethyl carbonate

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polybiphenyldimethyl Carbonate and Polydimethylsiloxane (PDMS) Composite

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ABSTRACT

Polymeric blends are useful in preparing hybrid materials with improved properties, related to packaging application. Blends are basically prepared with two or more than two polymers. The improvements in physical and chemical property of these blends are strongly depicted through their molecular level of interactions and therefore, guided by their mixing compatibility or homogeneity of the blends. To get the desired mechanical and gas barrier performance of the prepared polybiphenyldimethyl carbonate (PC) based packaging material, the optimum composition of PC with polydimethylsiloxane (PDMS) was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density was found to increase with the increase in poly (biphenyl dimethylcarbonate) fraction or lowing of polydimethylsiloxane fraction. The permeability properties of the blend were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases decreased with increase in mass fraction of biphenyl dimethyl carbonate. This in-silicostudy helps us to determine the best composition of the blend without performing laboratory experiments which saves valuable time and wastage of raw materials too.

Keywords: Gas permeability, Blend, in-silico analysis, Compatibility, Packaging

INTRODUCTION

Polymeric blends are usually offered improved physical and chemical properties like thermal, mechanical, gas barrier and biodegradability [1]. These properties are the prime interest for the researchers to design best packaging

material. Gas permeability is sometimes offered as essential criterion to design the polymer for biomedical and industrial utilization. For instance, polymers with high barrier properties, i.e. low permeability, are mandatory for food packaging applications to prevent loss of aroma, color and food-value and to slow down spoilage [2]. Apart from this food packaging application; there are lots of other applications which require the polymers to have high, low or tailored permeability like, filters and membranes for gas or liquid separation [3], protective coatings (e.g., paints and varnishes) [4], polymer coatings for controlled drug release [5] and water desalination [6].The permeability of liquids and gases through polymer membranes (plastic films) may be happened by either a temperature or pressure gradient, or by concentration gradient or external force field. The ''solution-diffusion'' mechanism is generally used to depict the pathway of gas permeation. It involvesthree steps. In the first step absorption of small molecules is happened into the membrane at the side of higher gradient (concentration, pressure, etc). On the other hand, second step involves the molecular diffusion through the membrane and the final step is related to desorption of those molecules from the membrane at the opposite side of lower gradient. The gas permeability in a polymer is generally varied with the nature of polymer and permeates. It may be accounted due to various degree of crystallinityand porosity of the polymers along with surface functionality (hydrophilic/ hydrophobic groups).

The main aim of combining polymeric materials is to achieve the desired quality of the material. Among various polymers, polybiphenyldimethylcarbonate (PC) is a widely used engineering plastics because of its physical and chemical properties like ductility, good thermal stability, excellent transparency, and high mechanical strength[7]. As a resultof these excellent properties, PC has been largely employed in electronic and electronic appliances along with automotive industry, having an annual production of 6 million tons. Recent report by Behboudi et. al. [8] shows thatPC is blended withpolyvinyl chloride (PVC)to preparethe ultrafiltration membrane for water purification. On the other hand, PC is also blended with poly(vinylidene fluoride) (PVDF) to prepare mechanically strong multicomponent nanocomposites with nanostructural reinforcement of graphenenanoplates, carbon nanotube, and organically modified montmorillonite [9]. In another recent report Wen et al. reinforced the graphene plates into blend of polybutyleneterethalate and polycarbonate [10] to obtain electrical and thermal conductive materials. The unique material, formed from the blend of PC with polystyrene is also reported to sense organic vapours with incorporation of multiwalled carbon nanotubes (MWCNTs) [11]. Polycarbonate blended polysulfone material is recently observed to have improved thermal and mechanical properties[12].

Therefore, investigation of blending compatibility of polycarbonate with other polymer is the urgent need of current research to develop advanced functional materials. All the above mentioned examples relied on laboratory experiments. Usually, preparation of homogeneous blend in wet-lab condition requires huge time and wastage of materials which can be minimized by in-silico approach through material studio [13] of "Biovia" software. In present context, we are focusing to optimize the homogeneous blend composition of poly (biphrnyl dimethylcarbonate) (PC) with polydimethylsiloxane (PDMS) in terms of gas permeability. Polydimethylsiloxane is a polymeric organosilicon compound, especially known for its unordinary rheological practices. Also it is optically clear, non-harmful and non-combustible. Polydimethylsiloxane (PDMS) shows wide applications like contact focal points, clinical gadgets and advanced elastomer materials. It is likewise utilized in creation of ointments and heat-resistant tiles. As of late, Adrees et. al. [14] prepared the PDMS based mixed layers with polyvinyl chloride-co-vinyl acetic acid derivative (PVCA) for CO_2seperation. Polydimethylsiloxane is likewise utilized in biomedical application like maxillofacial prosthetics, fake veins and articular ligament substitution, when it is mixed with poly (ether) ketone (PEEK) [15]. Consequently, the present in-silico approach towards examination of gas permeability of the blend having various composition of poly (biphenyldimethyl carbonate) (PC) and polydimethylsiloxane (PDMS) might be used to upgrade the sythesis to create attractive advanced materials for packaging applications.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systems of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction

Methodology

The structures of poly (biphenyl dimethylcarbonate) and polydimethylsiloxane (PDMS) were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of poly (biphenyl dimethylcarbonate) on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of poly(biphenyl dimethylcarbonate)and polydimethylsiloxaneas potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite increasedlinearly with increase in mass fraction of biphenyl dimethyl carbonate.

Density: Increase in density indicates decrease in porosity. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite increased linearly with increase in mass fraction of biphenyl dimethyl carbonates. Therefore, prepared materials offered compact structures which may not be suitable for adsorption, but suitable for packaging material, where high gas barrier property is required

Permeability of gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium.Lower permeability indicates longer time lag for the gas to pass through the membrane. Figure 3 shows that the permeability of oxygenthrough the hybrid polymer decreased with increase in mass fraction of biphenyl dimethyl carbonate.

On the other hand, Figure 4 shows that the permeability of nitrogenthrough the hybrid polymer is decreased with increase in mass fraction of biphenyl dimethyl carbonate.Thus the results indicated that an increase in biphenyl dimethyl carbonate fraction reduced the permeability of different gases. The rate of permeability might be influence by the molecular weight of the gases.

CONCLUSION

The possibility of use of poly (biphenyl dimethylcarbonate) and polydimethylsiloxaneto form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties.The molar volume and density decreased with increase in biphenyl dimethyl carbonate fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeabilityfor all the gases decreased with increase in mass fraction of biphenyl dimethyl carbonate. Usually components for a blend are identified experimentally. This in-silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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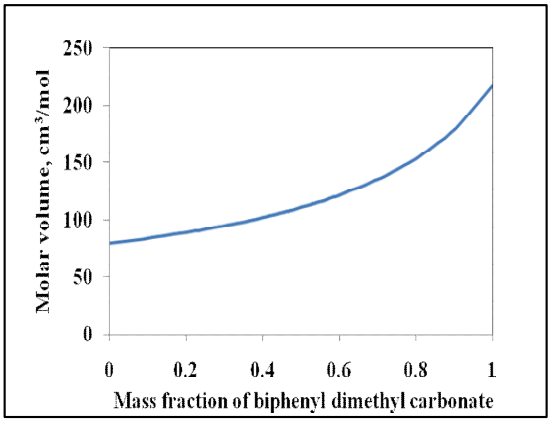

Figure 1. Change in molar volume with mass fraction of biphenyl dimethyl carbonate

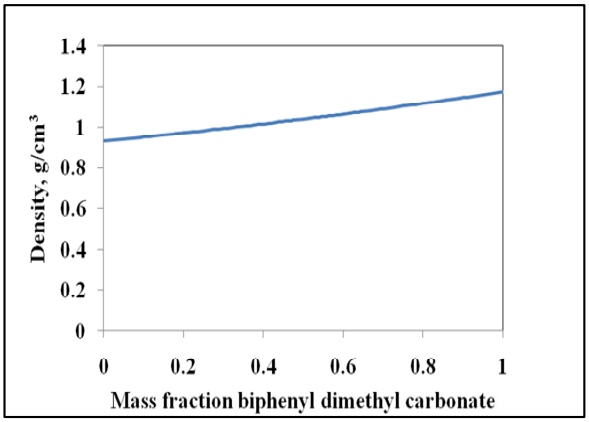

Figure 2. Change in density with mass fraction of biphenyl dimethyl carbonate

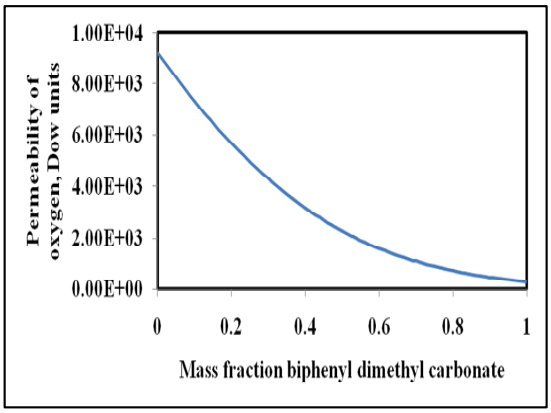

Figure 3. Change in permeability of oxygen with mass fraction of biphenyl dimethyl carbonate

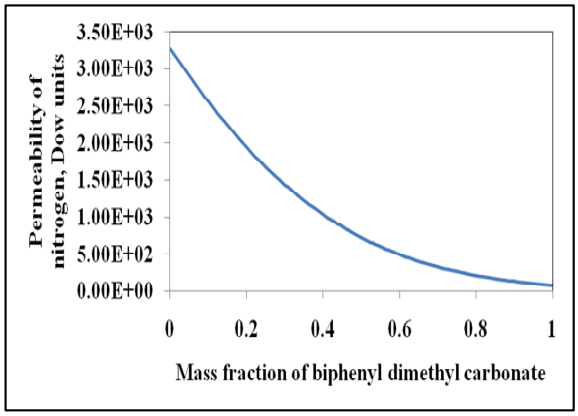

Figure 4. Change in permeability of nitrogen with mass fraction of biphenyl dimethyl carbonate

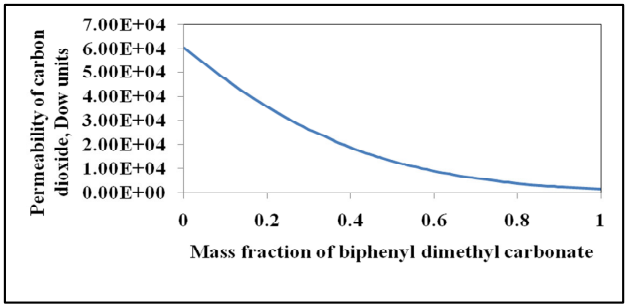

Figure 5. Change in permeability of carbon dioxide with mass fraction of biphenyl dimethyl carbonate

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyvinyl Alcohol and Poly-1, 2-α-D-Galactose Composite

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ABSTRACT

A blend is formed from the combination of two or more components. The change in properties of polyvinyl alcohol and poly-1, 2-α-D-galactose was studied to form a miscible blend using Biovia Materials Studio. The permeability properties of composition of the blend were studied so that it can be used in different potential application. The molar volume and density of the blend was observed to be decreased with increase in vinyl alcohol fraction. The permeability properties of the composite were observed based on permeability of various gases such as: carbon dioxide, nitrogen and oxygen. From analysis of results, it was noticed that the permeability property of these gases is decreased with increase in mass fraction of vinyl alcohol. This technique will be useful us to determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Blend; Biovia Material Studio; Gas permeability properties; Polyvinyl alcohol; In silico analysis

INTRODUCTION

Blends or composites are formed with combination of more than one component where components do retain their identity in the mixture. As it is incredibly tough to seek out multiple properties during a single material, it's suggested to mix totally different component thereby enhancing the properties of the material. Development of one material with the required property involves important analysis and time. A blend uses the upsides of various materials; blend them to get the ideal property. In this manner a blend spares time to build up a new material along with decreasing the cost of advancement of products with wanted properties. Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi-functional materials. Polymers combined with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber

composites [2] have been accounted for to upgrade mechanical properties and water resistance. Researchers have given attention on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can improve fire retardancy without expanding the weight [4]. Scientists have accentuated on synthesis and production of lightweight composite materials having high quality significant for upgrading fuel efficiency in the field of transportation [5]. There are uses of composites in structural Engineering because of high strength to weight proportion and resistance to corrosion. Consequently, glass fiber incorporated polymers, latex polymer cementations composites [6] were created for development of construction of bridges, light rail transit, mining and tunneling, holding dividers and other waterside buildings. All the previously mentioned models depended on research center analyses.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs.

Among different polymeric materials, polyvinyl alcohol (PVA) is one of the highly demanding material because of its robust and amicable properties such as: high dielectric nature, easy film formation ability, and adhesiveness properties. Moreover, the properties such material can be easily controlled according to requirement by altering the concentration of dopant [8, 9]. In the recent years, taking the advantages of PVA, many of the polymeric industry are inclined to produce strong polymeric films. These amicable properties of PAV have resulted in the formation of high mechanical strength and easy processability material [10]. In addition to that PAV is potentially non-toxic, biocompatible and easily soluble in water [11].

Researchers have used D-galactose in combination with other materials to different applications [12]. Poly-1, 2-α-D-galactose has been reported to be used in Curtius reaction. This study is intended to find out the change of gas permeability value of blend of polyvinyl alcohol and poly-1, 2-α-D-galactose with different proportions.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

The structures of polyvinyl alcohol and poly-1, 2-α-D-galactose were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly-1, 2-α-D-galactose as potential components of a composite was analyzed using Biovia Materials Studio. This computational tool uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate polymeric properties of materials. Furthermore, there are various computational methods belong to Group additive methods were extensively used from last few decades to determine the properties of polymer and small molecules. These computational methods are quite fast and pretty simple to use. Owing to these advantages, they have a great demand for rapid estimation of properties in critical condition without detailed understanding of the atomistic interactions. However, the principal shortcoming of these

methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated. To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar Volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Density: Increase in density indicates decrease in porosity. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Permeability of Gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium. Lower permeability indicates longer time lag for the gas to pass through the membrane. Figure 3 shows that the permeability of oxygen through the composite decreases with increase in mass fraction of vinyl alcohol.

Figure 4 shows that the permeability of nitrogen through the composite decreases with increase in mass fraction of vinyl alcohol. Figure 5 shows that the permeability of carbon dioxide through the composite decreases with increase in mass fraction of vinyl alcohol. Thus the results indicated that an increase in vinyl alcohol fraction reduces the permeability of different gases. The rate of permeability might be influence by the molecular weight of the gases.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly-1, 2-α-D-galactose to form a homogeneous blend was explored using Biovia Materials Studio. The molar volume, density and permeability of different gases such as oxygen, nitrogen and carbon dioxide were demonstrated using Biovia Materials Studio. From the results it was found that the molar volume and density decreased with increase in vinyl alcohol fraction. The permeability properties of the composites were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeability for all the gases decreased with increase in mass fraction of vinyl alcohol. Due to decrease in gas permeability value, the blend can be used in different practical application. Usually components for a blend are identified experimentally. This in silico study will help to determine components of a blend without doing experiments in laboratory.

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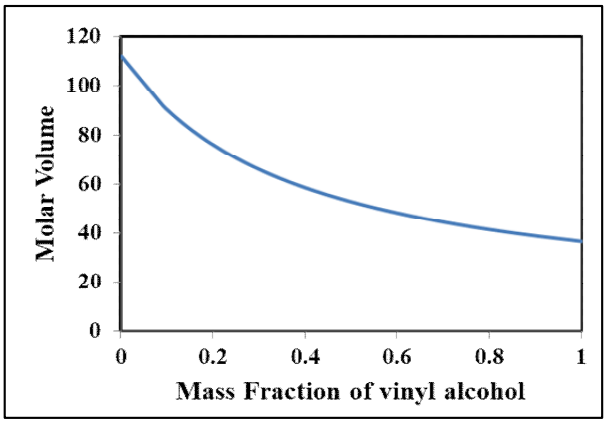

Figure 1. Change in molar volume with mass fraction of vinyl alcohol

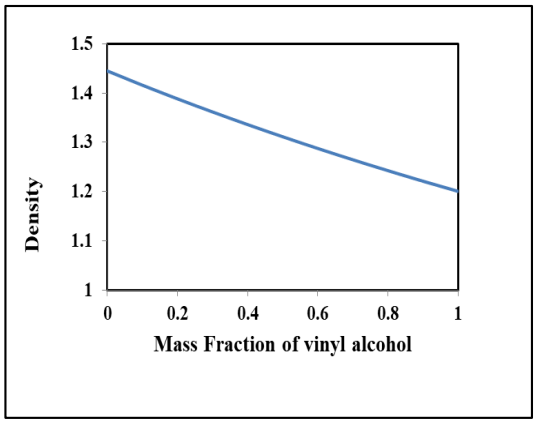

Figure 2. Change in density with mass fraction of vinyl alcohol

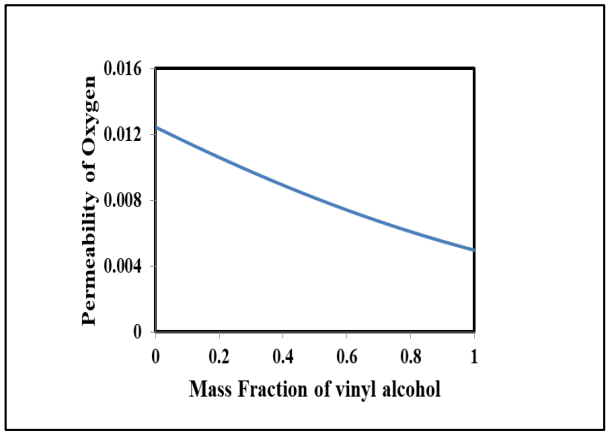

Figure 3. Change in permeability of oxygen with mass fraction of vinyl alcohol

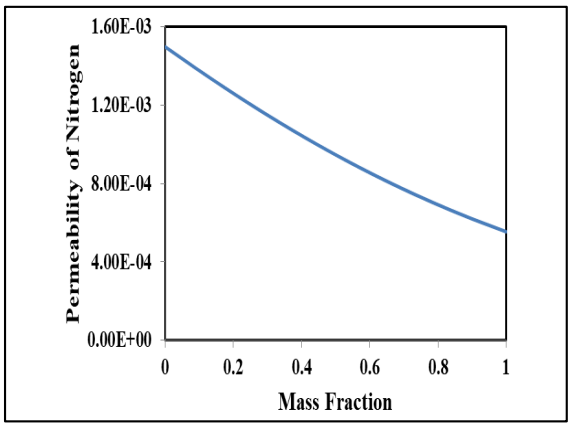

Figure 4. Change in permeability of nitrogen with mass fraction of vinyl alcohol

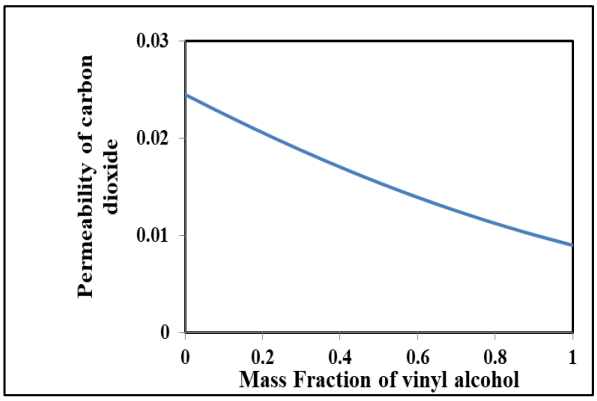

Figure 5. Change in permeability of carbon dioxide with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyvinyl Alcohol and Poly-1, 2-α-D-Glucose Composite

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ABSTRACT

The present work deals with the in silico information for mechanical properties of blend. These properties were determined by variation of polyvinyl alcohol and poly-1, 2-α-D-glucose compositions using Biovia, Materials Studio, Synthia analysis.Based on sheer, bulk, and Young's modulus and Poisson ratio, brittle stress fracture, the mechanical properties were determined.The results indicated that the values of bulk modulus, shear modulus, Young' modulus decreased with an increase in the mass fraction of vinyl alcohol whereas the Poisson ratio, and brittle stress fracture decrease. Usually, components for a blend are identified experimentally. This study will help determine pairs without performing laboratory experiments saving materials, money, and time.

Keywords: Synthia, in silico, polyvinyl alcohol, poly-1, 2-α-D-glucose, biovia material studio, mechanical property.

INTRODUCTION

The blend may be a homogenous or heterogeneous mixture. Blends or composites are the physical combinations of more than one component where components do retain their identity in the mixture. A single material cannot provide multiple anticipated properties. It is desirable to combine different components thereby improving the properties of the material. The development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus blending is a process that provides an easy pathway to develop a new material by reducing the cost of development of products with preferred properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer. The chemical and physical characteristics of a composite or blend are different from its constituents. Composites, usually are, matrices in which the distribution of reinforcement (strong/stiffness) is uniform [1-3]. The greater properties of composites are mainly due to their microstructure and interaction between the matrix and filler. [4, 5]. Polymers coupled with carbon-based (graphene, carbon nano-tube) nano-materials [6]

have drawn significant attention in recent years. Biodegradable polymers- natural fiber composites [7] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fireproof materials [8]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [9]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [10]. There are applications of composites in structural engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [11] were developed for the construction of bridges, light rail transit, mining, and tunneling, retaining walls, and other waterside buildings. All the above-mentioned examples relied on laboratory experiments.

Usually, blends are prepared by trial and error method and this technique is a low cost and less time-consuming method. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [12]) has been used to identify compatible pairs. The Polyvinyl alcohol (PVA) is a promishing material among various polymers, which is because of its easy film formation, high dielectric strength, good adhesiveness. These properties can be controlled by controlling the dopant concentration [13, 14]. The packaging industry widely uses the film forming ability of PVA forming strong film, which is because of environmental stability, greater mechanical strength , and easy processability [15]. In addition, PVA is non-toxic, hydrophilic, semicrystalline, easily soluble in water and biocompatible [16].

Different research groups have found applicability of glycopolymers (synthetic polymers containing pendant carbohydrate groups) for th removal of toxic chemicals and bacteria [17] Also it is used in in tumor cell recognition, and glucose-responsive insulin delivery [17]. Moreover, biopolymer blends possess good thermal stability [18]. By adding glycopolymers (cellulose nanoscale fillers) in different polymers (polyvinyl alcohol or polylactic acid) we can generate nanocomposites resulting in mechanical reinforcement and alternation of other properties [19].This study is intended to identify the interaction of polyvinyl alcohol and poly-12-a-D-glucose to form blends.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

The structures of polyvinyl alcohol and poly-1, 2-α-D-glucosewerefed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work, the use of polyvinyl alcohol and poly-1, 2-α-D-glucose as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. For the prediction of the properties of the polymers, group additive methods have been used from many years. The extreme fastness of these methods and easy usability makes them useful. Also their utility is high when a ripid estimation of a property is required. Without details of atomistic interactions. However, the important drawback of such methods is their dependability upon a database comprising of group contribution. Thus, if a polymer contains a group for which the

group contribution cannot be estimated, then the property of that polymer cannot be calculated. To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Bulk modulus: Bulk modulus is the measure of the decrease in volume with an increase in pressure. Figure 1 shows that the bulk modulus of the composite decreases linearly with an increase in mass fraction of vinyl alcohol.

Shear modulus: It is defined as the ratio of shear stress and shear strain. It shows the response of the composite to shear deformation. Figure 2 shows that the shear modulus of the composite decreases with increase in mass fraction of vinyl alcohol.

Young's modulus: It is defined as the ratio of stress and strain. It compares the relative stiffness of the composite. Figure 3 shows that Young's modulus of the composite decreases with increase in mass fraction of vinyl alcohol.

Poisson ratio: It is the ratio of lateral strain to longitudinal strain. Figure 4 shows that the Poisson ratio of the composite increases with increase in mass fraction of vinyl alcohol.

Brittle fracture stress: Brittle Fracture is the sudden, rapid cracking of a material under stress where the material exhibited practically no evidence of ductility or plastic degradation before the fracture occurs. Figure 5 shows that the brittle fracture stress of the composite increases with increase in mass fraction of vinyl alcohol.

CONCLUSION

The possibility of the use of polyvinyl alcohol and poly-1, 2-α-D-glucose to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed concerning mechanical properties. The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio, and brittle stress fracture. The findings show that the bulk modulus, shear modulus, YHoung'sjmodulus decreases with mass fraction of vinyl alcohol. On the other hand the Poisson ratio and brittle stress fracture decreases. The results indicated that the values of bulk modulus, shear modulus, Young' modulus decreased with an increase in the mass fraction of vinyl alcohol whereas the Poisson ratio, and brittle stress fracture decrease. Usually, components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money, and time.

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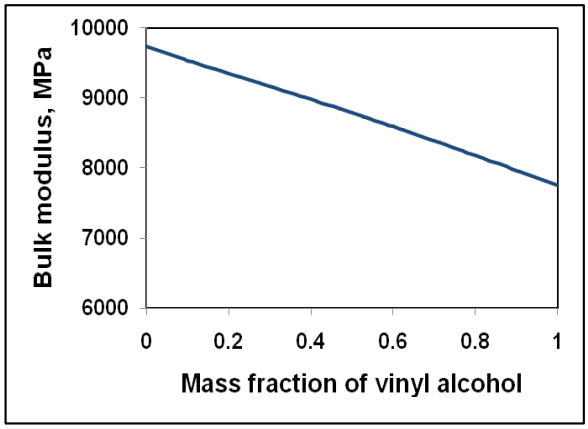

Figure 1. Change in bulk modulus with mass fraction of vinyl alcohol.

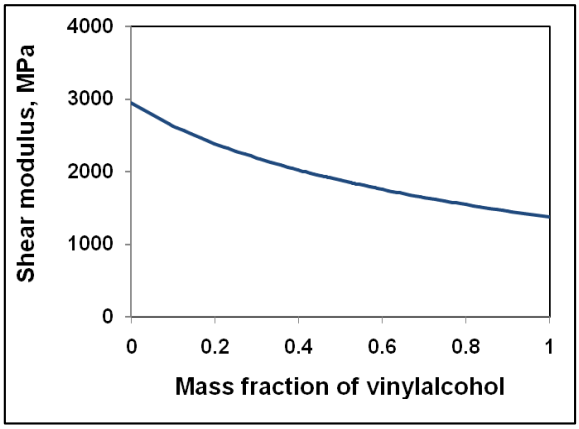

Figure 2. Change in shear modulus with mass fraction of vinyl alcohol.

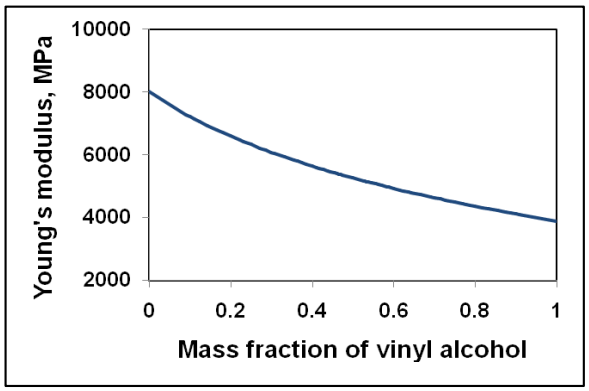

Figure 3. Change in Young's modulus with mass fraction of vinyl alcohol.

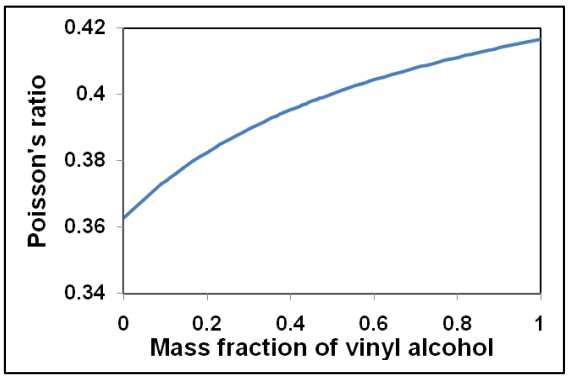

Figure 4. Change in Poisson modulus with mass fraction of vinyl alcohol.

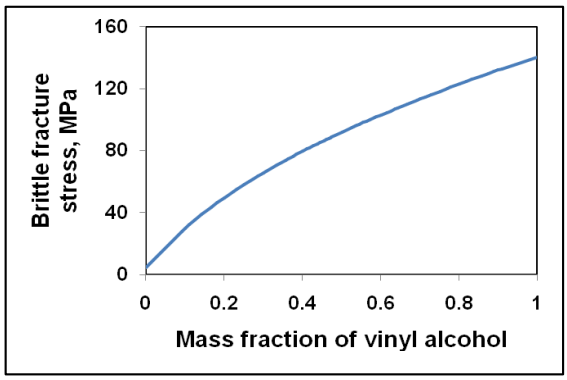

Figure 5. Change in brittle fracture stress with mass fraction of vinyl alcohol.

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RESEARCH ARTICLE

In silico Analysis of Polyvinyl Alcohol and Polyvinylchloride Compatibility in a Blend

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The selection of polyvinyl alcohol and polyvinylchloride to form a miscible blend was explored using Biovia Materials Studio. The compatibility of the two components was studied based on free energy of mixing, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible at and beyond 500K. Phase diagram indicated that a single phase can be obtained above 450 K which was the critical temperature. The coordination number was found to be 5.65 +/- 0.01. The highest number of configurations with respect to energy level was found to be -1.9 kcal/mol. The phase separation might lead to its use as porous material to be used as adsorbent. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: n silico analysis, blend, polyvinyl alcohol, phase diagram.

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance

flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money.Thus; researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs. Polymerization of monomers containing vinyl group leads to the formation of vinyl polymers such as polyvinyl chloride [8], poly styrene [9], polyvinyl esters[10], polyvinyl acetate[11, 12] etc. Polyvinyl alcohol (PVA) is a promising material among different polymers, because of its ability to form film easily, greater dielectric strength, good adhesiveness and also its properties can be tuned by concentration of dopant [13, 14]. Packaging industry widely uses the film forming ability of PVA, which is because of high mechanical strength, environmental stability and easy processability [15]. In addition, PVA hydrophilic, nontoxic, biocompatible and soluble in water [16].

Polyvinyl Chloride (PVC or Vinyl) find its applications in manufacture of medical devices, pipes, cable insulation, and wires and many others. It is known for superior mechanical and physical properties. However the fluid plasticity and thermal stability of PVC are inferior to those of other commodity plastics such as polyethylene and polystyrene [17]. Much work on improvement of the inferior properties of PVC has been carried out besides the addition of additives such as plasticizers, heat stabilizers, lubricants, fillers and other polymers [18]. This study is intended to identify the interaction of polyvinyl alcohol and polyvinyl chloride to form blends.

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

Polyvinyl alcohol and polyvinylchloride were prepared using the build menu of Materials Studio. The structure of the components were optimized using The components were used in blends->calculation menu of Materials studio. Polyvinyl alcohol was used as the base and polyvinylchloride was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend were analyzed.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and polyvinyl chloride as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where ΔG_m = Gibb's free energy of mixing

ΔH_m = Enthalpy of mixing

ΔS_m = *Entropyofmixing*

T = *Absolutetemperature*

The value of $T\Delta S_m$is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_malways depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$\Delta H_m < T\Delta S_m$ (2)

Figure 1 shows that the free energy involved in mixing is positive initially and then decreases gradually and attain even negative when the temperature moves from 50K to 500K. There is an exception seen in the phase diagram. When the temperature increased from 50K to 162.5K, the free energy of the process also increased which is against Eq. 1. Further increase in temperature decreased the free energy that supports Eq. 1. The result indicated that the blend will lead to a homogeneous mixture at and beyond 500K.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicates poor mixing. For chemically similar polymershaving small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains.Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similarcomponentsmaylead to a high positive value of χ (chi).

Figure 2 shows that the χ value is high for the temperature range studied (50 to 500 K) indicating demixing. The χ value decreased with increase in temperature. Thus at high temperature there is a possibility to form a miscible blend. The result is in agreement with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size.In this study the coordination number was found to be5.65 +/- 0.01.

Phase Diagram: The compatibility of binary mixtures can be visualized by phase diagrams. Figure 3 shows the phase diagram for the two components of the blend. There are three regions of different degree of miscibility:

a. The single-phase miscible region existed above the critical temperatureof around 450 K. This value supported the fact that a single phase blend can be formed at a moderate temperature (higher than 450 K) which is in agreement with the conclusion drawn from the free energy of mixing.

b. Fragmented metastable regions existedbetween binodals and spinodals, and

c. The two-phase separated regions of immiscibility are bordered by the spinodals.

The binodals separated miscible (one-phase) and metastable region, while the spinodals separated the metastable and two-phase region.

When the system enters from single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e, slow nucleation followed by growth of the phase separated domains.

On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 4 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreasedsignificantly. The maximum frequency was observed for the energy level of around -1.9kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 5 shows that the mixing energy for the system was high for the temperature range studied. The graph indicated that an increase in temperature helped reduce the mixing energy. This result supported the previous observations.

The formation of nonhomogeneous blend with polyvinyl alcohol as base might help formation of blend with higher porosity such as hydrogel. This might have an application as adsorbent.

CONCLUSION

The possibility of use of polyvinyl alcohol and polyvinyl chloride to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible at a temperature of 500K or more than that. Phase diagram indicated that a single phase can be obtained above 450 K. The coordination number was found to be 5.65 +/- 0.01. The maximum number of configurations with respect to energy level was found to be -1.9kcal/mol.The phase separation might make it a porous material to be used as an adsorbent. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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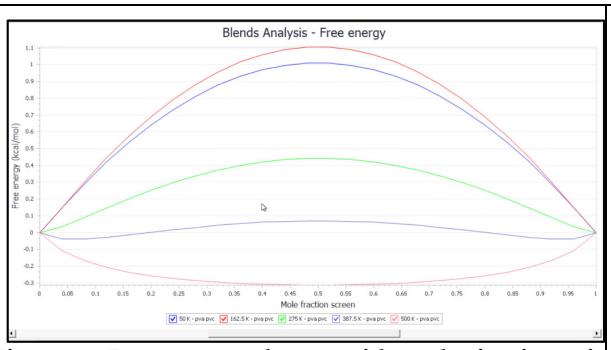

Figure 1. Free energy change with mole fraction of polyvinyl chloride at different temperature

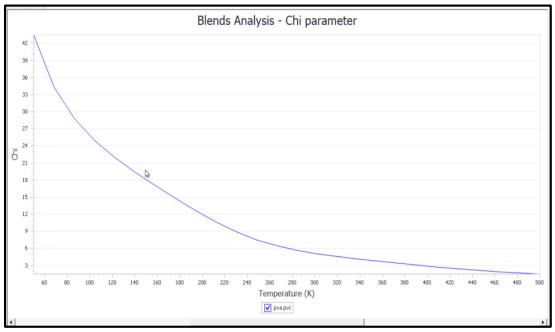

Figure 2. Change in χ (chi) value with temperatu

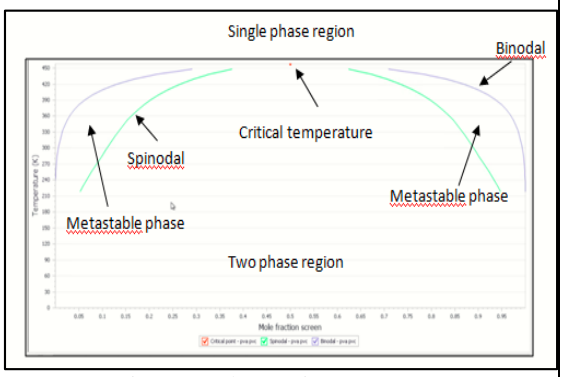

Figure 3. Phase Diagram

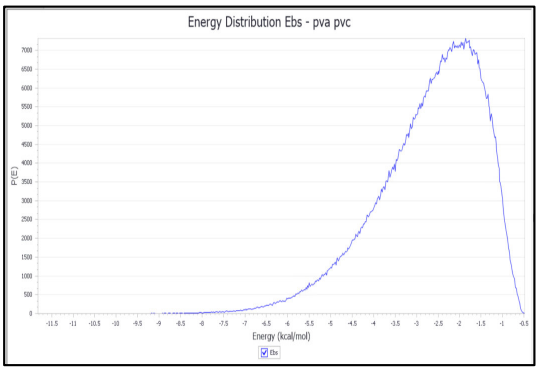

Figure 4. Energy Distribution

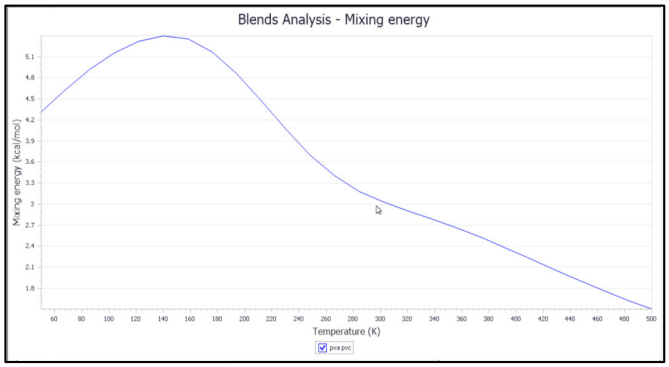

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyacrylic Acid and Polyurea Compatibility in a Blend

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ABSTRACT

A blendis especially to combine or associate of more than one constituents or the line of demarcation cannot be distinguished. The desired property of a blend is its homogeneity. The selection of polyacrylic acid and polyurea to form a miscible blend was explored using Biovia Materials Studio. The compatibility of the two components was studied based on the free energy of mixing, chi parameter, phase diagram, and mixing energy. The results indicated that the pair can become compatible only at high temperatures. Phase diagram indicated that a single phase can be obtained above 750 K which was the critical temperature. The coordination number was found to be 5.36 +/- 0.04. The highest number of configurations concerning energy level was found to be -1.4 kcal/mol. The phase separation might lead to its use as porous material to be used as adsorbent. This study will help determine pairs without performing laboratory experiments saving materials, money, and time.

Keywords: Blend, in silico, polyacrylic acid,polyurea

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. The development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.Nanomaterial modified polymers paved the way for multifunctional materials. Polymers coupled with carbon-based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fireproof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame

retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for the construction of bridges, light rail transit, mining and tunneling, retaining walls, and other waterside buildings. All the above-mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials; time, and money.Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Acrylic polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects, etc. [8], bone repair [9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc.[10].

Polyacrylic acid is a polyelectrolyte soluble in aqueous media at neutral pH It is used for preparing hydrogels. It is not toxic and does not irritate [11]. This study is intended to identify the interaction of polyacrylic acid and polyurea to form blends. Polyurea, which is a typical elastomer, is a reaction product of an isocyanate and a synthetic resin blend through polymerization step growth. The isocyanate can be monomer, polyhmer, aliphatic or aromatic. It can also be any variant reaction of of isocyanates, quasi-prepolymeror a prepolymer. The prepolymer /quasi-prepolymer may be a hydroxyl-terminated polymer or an amine-terminated [12].

MATERIALS AND METHODS

Software Used

Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology

Polyacrylic acid and polyurea were prepared using the build menu of Materials Studio. The structure of the components was optimized using the components that were used in the blends->calculation menu of Materials studio. Polyacrylic acid was used as the base and polyurea was used as a screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acid and polyurea as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where $\Delta G_m = Gibb's\ free\ energy\ of\ mixing$

$\Delta H_m = Enthalpy\ of\ mixing$

$\Delta S_m = Entropy\ of\ mixing$

$T - Absolute\ temperature$

The value of $T\Delta S_m$is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_malways depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$\Delta H_m < T\Delta S_m$ (2)

Figure 1 shows that the free energy involved in mixing is always positive for the temperatures studied. The free energy decreases with an increase in temperature as evident from Eq. 1. The results indicated that the blend will not lead to a homogeneous mixture for the temperature range studied (50 to 500 K). The trend suggested that there might be a possibility of a miscible blend at a very high temperature.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicates poor mixing. For chemically similar polymershaving small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains.Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similarcomponentsmaylead to a high positive value of χ (chi).

Figure 2 shows that the χ value is high for the temperature range studied (60 to 480 K) indicating demixing. The χ value decreased with an increase in temperature. Thus at high temperature there is a possibility to form a miscible blend. The result is in agreement with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It assumed that molecules that are not arranged on a regular lattice is expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size.In this study the coordination number was found to be 5.36 +/- 0.04.

Phase Diagram: The compatibility of binary mixtures can be visualized by phase diagrams. Figure 3 shows the phase diagram for the two components of the blend. There are three regions of different degree of miscibility:
a. The single-phase miscible region existed above the critical temperatureof around 750 K. This value supported the fact that a single-phase blend can be formed at a high temperature (higher than 750 K).
b. Fragmented metastable regions existedbetween binodal and spinodals, and
c. The two-phase separated regions of immiscibility are bordered by the spinodals.
The binodal separated miscible (one-phase) and metastable region, while the spinodals separated the metastable and two-phase region.When the system enters from a single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e, slow nucleation followed by growth of the phase-separated domains. On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 4 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations

with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -1.4kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 5 shows that the mixing energy for the system was high for the temperature range studied. The graph indicated that an increase in temperature helped reduce the mixing energy. This result supported the previous observations. The formation of a nonhomogeneous blend with polyacrylic acid as a base might help the formation of blend with higher porosity such as hydrogel. This might have an application as adsorbent.

CONCLUSION

The possibility of the use of polyacrylic acid and polyurea to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on the free energy of mixing, chi parameter, phase diagram, and mixing energy. The results indicated that the pair can become compatible at high temperatures. Phase diagram indicated that a single phase can be obtained above 750 K. The coordination number was found to be 5.36 +/- 0.04. The maximum number of configurations concerningthe energy level was found to be -1.4 kcal/mol.The phase separation might make it a porous material to be used as an adsorbent. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money, and time.

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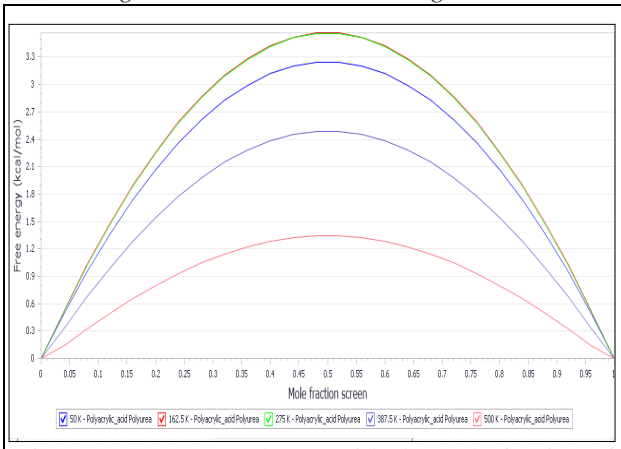

Figure1. Free energy change with the mole fraction of polyurea at different temperatures

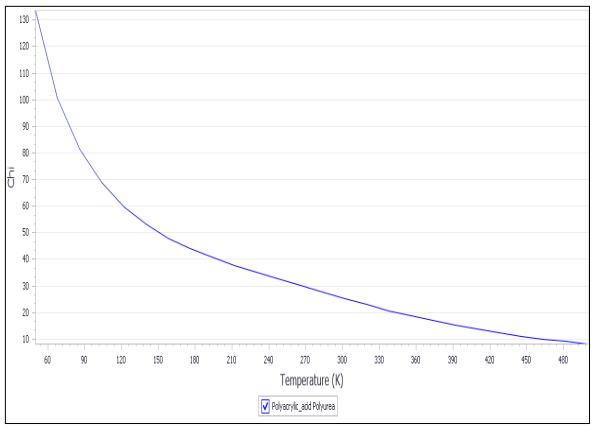

Figure 2. Change in χ (chi) value with temperature

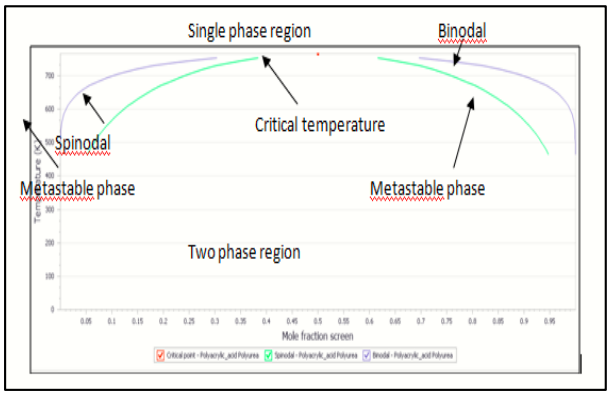

Figure3. Phase diagram

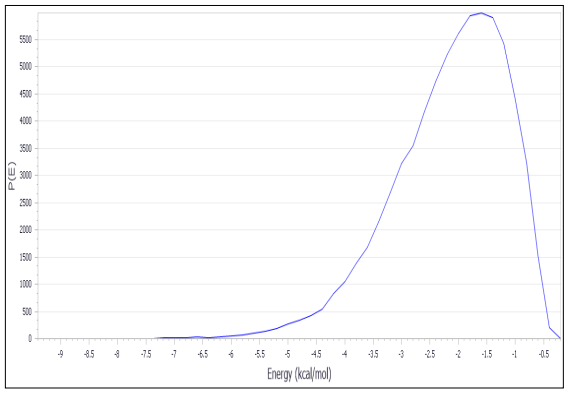

Figure4. Energy distribution

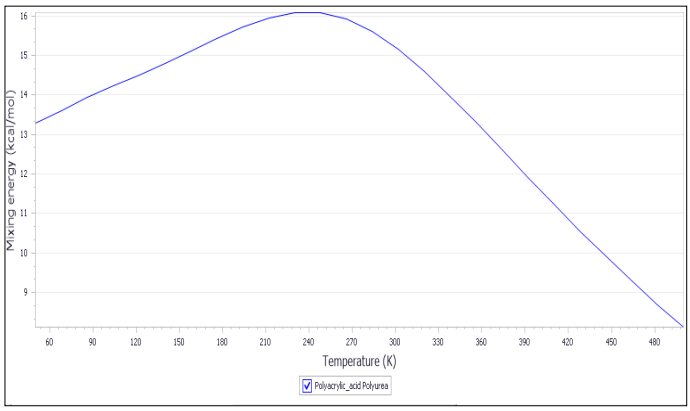

Figure5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyvinyl Alcohol and Polyvinyl Chloride Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The two parameters excluding heat capacity are found to be increasing but heat capacity itself decreased with the rise in the value of mass fraction of vinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: In-silico analysis, polyvinyl chloride, thermal property, composite, dielectric property, polyvinyl alcohol

INTRODUCTION

Blends or composites are materials containing more than one components. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio

and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs.

There exist different vinyl polymers which are formed by the polymerization of the monomers that contains vinyl groups. Some of these vinyl polymers are namely polyvinyl chloride [8], poly styrene [9], polyvinyl esters [10], polyvinyl acetate [11, 12] etc. Polyvinyl alcohol (PVA) has high dielectric strength, easy film formation and adhesiveness for which it is treated as a novel material among various polymer materials. By varying the dopant concentration, the above properties can also be controlled [13, 14]. Strong polymeric films are fabricated by packaging industries using the film forming ability of PVA. This is possible due to some of the interesting properties of PVA such as easy processability, high mechanical strength and environmental stability [15]. PVA finds its use in different industries and it is a semicrystalline, non-toxic, and hydrophilic material which is also biocompatible and easily soluble in water [16].

Manufacturers use Polyvinyl Chloride (PVC or Vinyl) for the production of pipes, medical devices, wire and cable insulation due to its high strength thermoplastic material property. PVC has superior mechanical and physical properties for which it is the leading synthetic plastic polymer having third-largest production in the world. But, materials like polyethylene and polystyrene used as commodity plastics show better fluid plasticity and thermal stability than PVC [17]. For the improvisation of the above properties, research work has been carried out which excludes many handy experiments. These experiments are comprised of the addition of additives like plasticizers, heat stabilizers, lubricants, fillers and other polymers to PVC to uplift the desired properties [18]. The present study is focused on the formation of blends by identifying the interaction of polyvinyl alcohol and polyvinyl chloride with each other.

MATERIALS AND METHODS

Software Used

The analysis was carried out by using the *Materials studio* module of *Biovia software* (*Dassault Systemes of France*). Techniques like machine learning and standard algorithms are utilized by the software to predict the level of interaction.

Methodology

The structures of PVA and PVC were fed to the *synthia* menu of *Materials Studio*. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and polyvinylchloride as potential components of a composite was analyzed using Biovia Materials Studio. Wide range of polymer properties can be evaluated by BIOVIA Materials Studio Synthia using pre-defined correlations (advanced quantitative structure-property relationships). The properties of polymers along with small molecules were predicted by using *Group additive methods* for many years which are supposed to be extremely fast and easy to use. These methods are of great utility for rapid estimation of

any property of a material. This can be processed without a detailed understanding of the atomistic interactions which give rise to the specified property. But, there exist a major drawback of these methods which is nothing but the dependence of these methods on a database of group contributions. So, the property of a polymer cannot be calculated if it contains a group for which the group contribution cannot be estimated.

Synthia (Biovia) uses the topological information about the polymers in the predictive correlations and implementation of this method helps in overcoming the above limitation. Here, graph theory used to derive the connectivity indices is employed and there is no requirement of any database of group contributions. The properties of any polymer constituted by these nine elements such as; carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine and bromine can be predicted by the above method.

Heat capacity: Without changing the phase, the amount of heat needed to raise the temperature by 1°C of one unit weight of a substance is called heat capacity. Figure 1 shows that the heat capacity (Cp) of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Thermal conductivity: It indicates the correlation between heat flux per unit area and temperature gradient. It refers to the intrinsic ability of a material to transfer heat. Figure 2 shows that the thermal conductivity of the composite linearly increases with increasing value of mass fraction of vinyl alcohol.

Dielectric constant: The dielectric constant of a material may be defined as the ratio of the electric permeability of the material to the electric permeability of free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant. Figure-3 shows that the dielectric constant of the composite linearly increases with increasing value of mass fraction of vinyl alcohol.

CONCLUSION

The possibility of use of polyvinyl alcohol and polyvinylchloride to form a blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. As per the result, the values of thermal conductivity and dielectric constant increases with increasing value of mass fraction of vinyl alcohol except heat capacity. Heat capacity for the blend shows a decreasing trend with increasing value of mass fraction of the base taken. Usually, components for a blend are identified experimentally. This in-silico study will help in determining the components of a blend without performing laboratory experiments saving materials, money and time.

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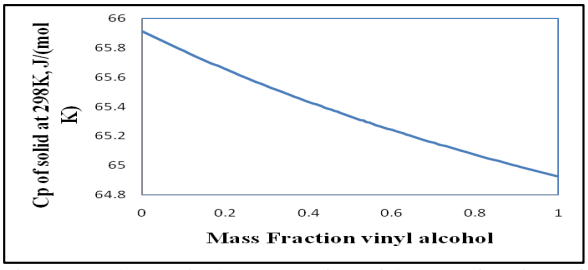

Figure 1. Change in heat capacity with mass fraction of vinyl alcohol

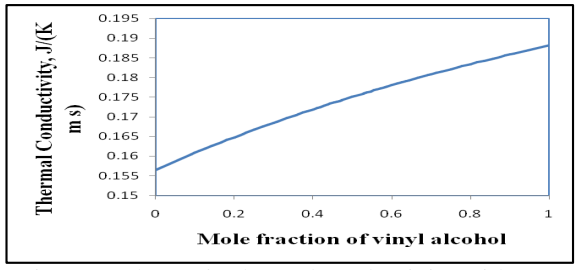

Figure 2. Change in thermal conductivity with mass fraction of vinyl alcohol

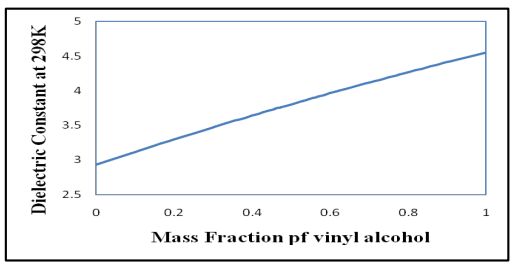

Figure 3. Change in dielectric constant with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Blend Compatibility Investigation of Poly (Biphenyl Dimethyl Carbonate) and Poly (Ether Sulfone)

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ABSTRACT

Polymeric blend having two or more components is the easiest and low cost way to generate hybrid polymer with improved properties. Strong molecular interaction in homogeneous blend is the key to enhance the physical and chemical properties of polymers. In this manuscript, we have tried to explore the compatibility of poly (biphenyl dimethylcarbonate) and poly(ethersulfone) to form a miscible blend using Biovia Materials Studio. The blending compatibility of these two polymers was studied based on free energy of mixing, phase diagram, chi parameter, and mixing energy. The obtained results depicted the immiscibility of these two polymers in the temperature range of 50 K to 500 K. However, higher temperature may lead the miscibility condition, as revealed from phase diagram. The coordination number was found to be 5. The highest number of configurations with respect to energy level was found to be -2.1 kcal/mol. This study may help in determining the optimal composition of pairs and temperature for the preparation of homogeneous blend without performing laboratory experiments and therefore, saving materials, money and time.

Keywords: Blend, in silico, biphenyl dimethylcarbonate, ether sulfone

INTRODUCTION

The current age is essentially managing the improvement of existing one in all areas of science and technology. Polymers are structurally designated with large molecular weight entities, having propagation of repeating units. It shows a reiteration in their separated auxiliary units and notable for their capacity to be used in day by day needs [1]. The much of the time utilized technique for altering the properties of polymers is their mixing with other polymers and it prompts the improvement in different properties like thermal [2], mechanical [3] and electrical properties [4]. The arrangement of miscible mixes permits most obviously changing the properties of polymers; nonetheless, there are not all that numerous sets of polymers shaping such mix [5]. In many cases, polymers are miscible just on account of a low proportion of one of them, or they are low- molecular weight or because of a proper

choice of the compatibilizer [6]. From the thermodynamic perspective, miscibility of a blend relies on the decline of Gibbs free energy of blending and identified with change in entropy and enthalpy. Subsequently, the examination of blending compatibility of two or more polymeric components is the essential parameter to plan hybrid polymers with improved properties. Besides, with the ongoing situation, hybrid polymers are broadly utilized with nanostructural filler (carbon nanotube, nanoclay, graphene, and so forth.) to convey magnificent properties, for example, electrical or semiconducting [7], thermal [8] and mechanical properties [9]. Among different polymers, polybiphenyldimethylcarbonate (PC) is a widely used engineering plastics because of its physical and chemical properties like ductility, good thermal stability, excellent transparency, and high mechanical capacity [10]. Because of these phenomenal properties, PC has been to a great extent utilized in electronic and electronic machines alongside car industry, having a yearly creation of 6 million tons. Ongoing report by Behboudi et. al.

[11] shows that PC is mixed with polyvinyl chloride (PVC) to set up the ultrafiltration film for water filtration. Then again, PC is additionally mixed with poly(vinylidene fluoride) (PVDF) to get ready precisely solid multicomponent nanocomposites with nanostructural enrichment of graphenenanoplates, carbon nanotube, and naturally adjusted montmorillonite [12]. In another report Wen et al. incorporated the graphene plates into mixture of polybutyleneterethalate and polycarbonate [13] to acquire electrical and thermal conductive materials. As per the literature review, a advanced sensing material was framed from the blend of PC with polystyrene to detect organic vapors with inclusion of multiwalled carbon nanotubes (MWCNTs) [14]. Polycarbonate mixed polysulfone material was reported with improved thermal and mechanical properties.[15].Therefore, examination of blending capability of polycarbonate with other polymer is the pressing need of ebb and flow research to create progressed useful materials. All the previously mentioned models depended on lab tests. For the most part, readiness of homogeneous mix in wet-lab condition requires colossal time and wastage of materials which can be limited by in-silico approach through material studio [16] of "Biovia"software. In present context, we are focusing to optimize the homogeneous blend composition of polybiphrnyldimethylcarbonate (PC) with poly(ether sulfone) (PES). Among various engineering polymers, polyether sulfone (PES) is a high-temperature sustaining thermoplastic polymer with striking strength and chemical stability from various organic solvents. It belongs to the polysulfone family and contains an aryl-SO_2 subunit in their long chain structures. Nonetheless, the intrinsic hydrophobic property of PES formulatesthis prepared material sensitive to membrane fouling, restricting its more wide-rangingrelevance in water treatment based on membrane. Due to high chemical stability it is also preferably used for gas separation in harsh environment. To improve the gas separation efficiency of PES, a few investigations have been performed. In a report, Adib et al. [17] incorporated the nanostructural silica to improve the gas separation.

However, blending of PES with other hydrophilic polymer is one of the easiest routes to improve the efficiency of the gas separation. In another report, Mannan et al. [18] explored the gas-permeation behavior of glassy poly(vinyl acetate) (PVAc)–PES hybrid films and PSF–PES film. Interestingly, it is found that the gas permeation properties of hybrid PSF–PES film is remain unaltered as compared to the properties of polyether sulfone. However on account of the PES–PVAc hybrid polymer, low selectivity was observed for gas separation and may be accounted as the phase separation in their blend. Kamal et al. [19] revealed that the blend with elastomers (like polydimethylsiloxane) leads to the improved gas penetration properties of the polydimethylsiloxane–PES hybrid. Akbarian et al.[20] prepared the PES based blend membranes for CO_2 gas separation with inclusion polyethylene glycol (PEG) as second polymer [20]. Therefore, the present in-silico approach of blend analysis between polybiphenyl dimethyl carbonate (PC) and polyether sulfone(PES) may be utilized to optimize the composition to fabricate desirable functional materials with some improved physical and chemical properties.

MATERIALS AND METHODS

Software Used: In this study different tools of Bioviasoftware (Materials studio) (Dassault Systemes of France) was used for this blend analysis. The software used the machine learning techniques and standard algorithms to calculate the mode of interaction.

Procedure: Poly (biphenyl dimethylcarbonate) and poly (ether sulfone) were prepared using the build menu of the Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polybiphenyl dimethyl carbonate was used as the base and poly (ether sulfone) was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed in order to gain knowledge regarding the compatibility of the components to form a blend.

RESULTS AND DISCUSSION

In this investigation, we have used polybiphenyldimethylcarbonate (PC) and poly(ether sulfone) as potential components of a blend and it was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

Where, ΔG_m — *Gibb's free energy of mixing*

ΔH_m = *Enthalpy of mixing*

ΔS_m = *Entropy of mixing*

T = *Absolute temperature*

The value of $T\Delta S_m$ is always positive in case of a blend, when entropy of mixing increases . As a result, the positive and negative sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. A miscible blend can be formed by the components when the free energy entropic contribution exceeds the enthalpic contribution, i.e.,

$$\Delta H_m < T\Delta S_m \quad (2)$$

Figure 1, shows that the free energy involved in mixing is positive for all values of temperature, indicating the phase separation in the entire range of temperature. However, higher temperature may satisfy the condition of forming a single phase for these two polymeric components.

Phase Diagram: Fig. 2 represents the phase diagram of the blend having poly (biphenyl dimethyl carbonate) (PC) and polydimethylsiloxane (PES) in their composition. Phase diagram is particularly helpful in predicting the different region of varying miscibility in connection to the temperature and composition. In present figure 1200 K shows the upper critical solution temperature (UCST) above which single phase miscible region is observed. Fragmented metastable region is observed in between bimodal (blue lines) and spinodal lines (green lines). The region of phase separation is underlined by spinodal, whereas, binodalseperates the single-phase and meta-stable region. Again the system enters from single-phase state to the metastable state, the phase separation usually occurs by the mechanism of resembling crystallization i.e, slow nucleation along with growth of the phase separated domains. On the other hand, spinodal decomposition mechanism happens when the system leaps from a single-phase into the spinodal state of immiscibility the phases separate spontaneously.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicates poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similar components may lead to a high positive value of χ (chi). Figure 2 shows that the blend of PC and PES has basically depicted the positive values of χ (chi) within a

temperature range of 50 K to 500 K. It confers the de-mixing of these two polymeric components due to mismatching of their cohesive in the entire range of temperature, studied. Therefore, represents a state of phase separation. However, poly (biphenyl dimethyl carbonate) (PC) and poly (ether sulfone) (PES) are not mixed to form a homogeneous blend in wide range of temperature and the data is well supported from the free energy of mixing of the blend.

Coordination Number: The coordination number Z_{ij} is defined as the number of molecules of type *j* that can be crowded around a single molecule of type *i*. The coordination number was determined for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It is understood that molecules which are not aligned on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size. In this study the coordination number was found to be 5.

Energy Distribution for Blend: Fig.4 shows the variation of population of different energy levels associated with pair having different configuration and orientation. It shows that the distribution is broad in nature. Maximum molecular population is observed to be centered around -2.1 kcal/mol, and distribution around this value is asymmetric in nature. As expected majority of pair configuration lies on the low energy value to attain a stable state.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low may be suitable for mixing. Figure 5 shows that the mixing energy for the system was small (19.5 kcal/mol) for the temperature range 50K-270 K. Afterward, increase in temperature leads to the higher values of free energy which eventually leads to the conclusion of phase separation at higher temperature. But at low temperature (50K-270K), mixing may be possible due to small positive values of free energy.

CONCLUSION

The possibility of use of polybiphenyl dimethyl carbonate and poly (ether sulfone) and to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair can have very good compatibility at different ranges of temperature. The coordination number was found to be 5. The maximum number of configurations with respect to energy level was found to be -15 kcal/mol. usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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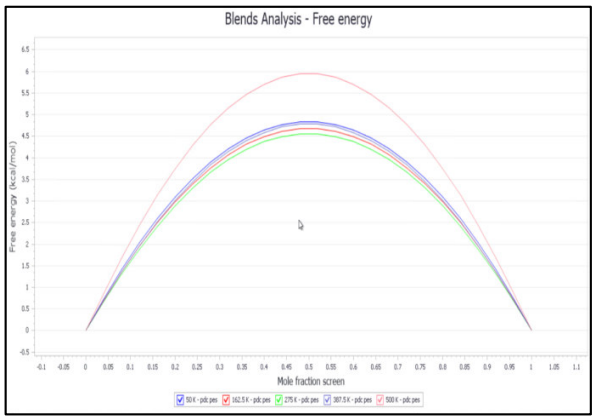

Figure 1. Free energy change with mole fraction of poly(ether sulfone) at different temperatures

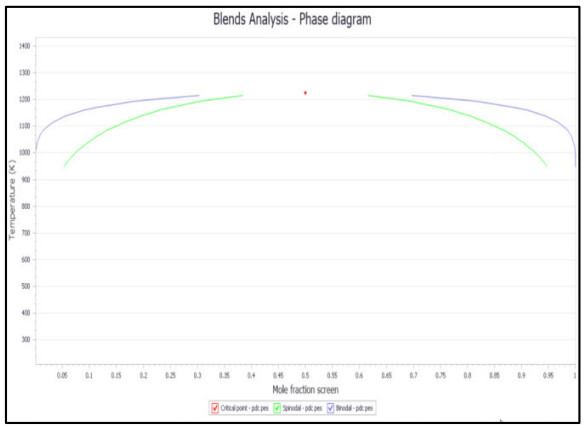

Figure 2. Phase diagram of the blend

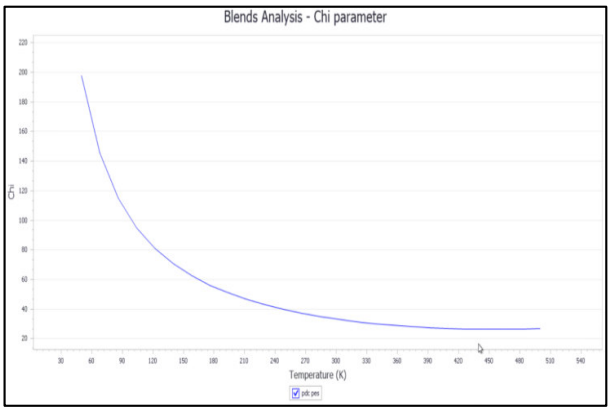

Figure 3. Change in χ (chi) value with temperature

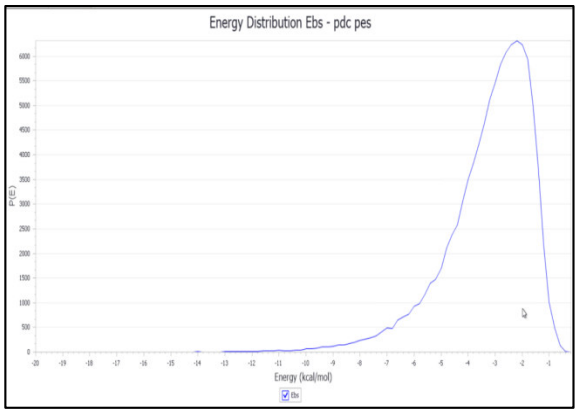

Figure 4. Energy distribution

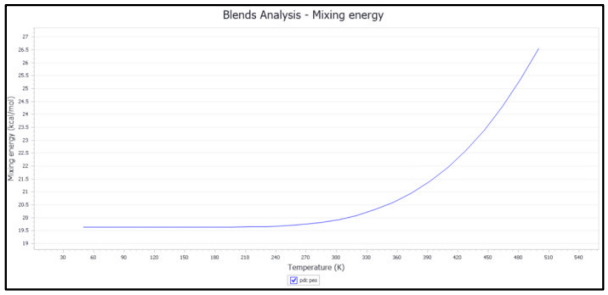

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyvinyl Alcohol Acid and Poly-1, 2-α-D-Glucose Compatibility in a Blend

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ABSTRACT

In this work the compatibility of polyvinyl alcohol and poly-1, 2-α-D-glucose was studied to form a miscible blend using Biovia Materials Studio blend analysis.The combination of two or more components is said to be a blend. The compatibility of the two components was demonstrated based on free energy of mixing, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible only at high temperature. The phase diagram indicated that a single phase can be obtained above 460 K which was the critical temperature. The coordination number was found to be 6.85 +/- 0.04. The highest number of configurations with respect to energy level was found to be -2.0 kcal/mol. This study will not only help to determine pairs without performing laboratory experiments but also less time consuming and low cost process.

Keywords: Blend, in silico, polyvinyl alcohol, poly-1, 2-α-D-glucose, biovia material studio.

INTRODUCTION

The blend may be a homogenous or heterogeneous mixture. Blends or composites are the physical combination of more than one component where components do retain their identity in the mixture. A single material cannot provide multiple anticipated properties. It is desirable to combine different components thereby improving the properties of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus blending is a process which provides an easy pathway develop a new material by reducing the cost of development of products with preferred properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer. A composite/blend exhibit significantly diversephysic –chemical characteristics from those of its constituent components. In a composite the constituents remain physically separable and different from each other. Generally, a composite is a matrix materialwhere strong and stiff reinforcement is dispersedwith a soft and weaker components interaction [1-3].As repoted the enhanced properties of composites are mostlyaffected by their

microstructure and contact between matrix and reinforcing materials in the inter-phase state [4, 5].Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [6] have drawn significant attention in recent years. Biodegradable polymers- natural fiber composites [7] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [8]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [9].

Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [10]. There are applications of composites in structural engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [11] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.Usually blends are prepared by trial and error methodandthis technique is a low cost and less time consuming method. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [12]) has been used to identify compatible pairs.

With all this available s polymers, polyvinyl alcohol (PVA) is a potential candidate due to its physical properties like high dielectric strength, easy film formation, adhesiveness [13, 14]. The polymer properties can be tuned by incorporating various impurities particle. PVA has very unique film forming ability which leads the material to packaging industry to form strong polymeric films due to its high mechanical strength, environmental stability and easy fabrication [15]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [16].

Researchers have found many applications of glycopolymers (synthetic polymers containing pendant carbohydrate groups) in the field of biology like toxic removal from body, drug delivery, insulin delivery[17]. It has been found that biopolymer blends possess good thermal stability [18].By adding glycopolymers (cellulose nanoscale fillers) in different polymers (polyvinyl alcohol or polylactic acid) we can synthesize nanocompositeshaving mechanical reinforcement and alternation of other properties [19].This study is intended to identify the interaction of polyvinyl alcohol andpoly-1, 2-α-D-glucose to form blends.

MATERIALS AND METHODS

Software Used: Biovia software with various tools and techniques (Dassault Systemes of France) was used for analysis. The standard algorithms along with machine learning techniques were used to predict the level of interaction.

Methodology: Polyvinyl alcohol and poly-1, 2-α-D-glucose were prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyvinyl alcohol was used as the base and poly-1, 2-α-D-glucose was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly-1, 2-α-D-glucose as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

Where $\Delta G_m = Gibb's free energy of mixing$

$\Delta H_m = Enthalpy of mixing$

$\Delta S_m = Entropy of mixing$

$T = Absolute temperature$

The value of $T\Delta S_m$ is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$$\Delta H_m < T\Delta S_m \quad (2)$$

Figure 1 shows that the free energy involved in mixing are negative at around 160 Kandbeyong 500 K and positive for other temperature regeions studied here. The free energy decreases with increase in temperature (upto160 K) as evident from Eq. 1 and free energy increases with increase in temperature after 165 K upto 330 K.Furthet increase in the temrature it decreases gradually. The results indicated that the blend will lead to a homogeneous mixture for the temperature around 161 K and beyond 500 K. The trend shows a very good compatibility between polyvinyl alcohol and poly poly-1, 2-α-D-glucose with negative value of mixing energy for the above mentioned temperatures, which may form a perfect blend with significantly less effort.

Chi Parameter: The Flory–Huggins χ parameter explains the excess free energy of mixing and helps to identify the phase behavior for blending of polymers and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicates poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demising for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similar components may lead to a high positive value of χ (chi).

Figure 2 shows that the χ value is high or low for the low and high temperature range (500 K) respectively indicating mixing of the components at high temperature. The χ value decreased with increase in temperature. Thus at high temperature a miscible blend may be formed. This agrees with the free energy of mixing for the blend.

Coordination Number (CN): The coordination number Z_{ij} is the number of molecules of type *j* that can be surrounded by a single molecule of type *i*. The CN was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used for lattice calculation. It is predicted that molecules are not followed on a regular lattice mode as expected in the original Flory-Huggins theory. The coordination number is useful only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pair's method in defining a coordination number for a binary system in which the components are not similar in size. In this study the coordination number was found to be 6.85 +/- 0.04.

Phase Diagram: The compatibility of binary mixtures can be obtained by phase diagrams. Figure 3 shows the phase diagram for the two components of the blend. There are three regions of different degree of miscibility:

a. The single-phase region which is shown miscible lies above the critical temperature of around 460 K. This value indicated the fact that a single phase blend can be formed at a high temperature (higher than 460K).

b. Fragmented metastable regions existed between binodals and spinodals, and

c. The two-phase separated regions of immiscibility are bordered by the spinodals.

The binodals separated miscible (one-phase) and metastable region, while the spinodals separated the metastable and two-phase region.

When the system enters from one of the single phase region to the other metastable region, resembling crystallization of phase separation play an important role which is the slow nucleation followed by growth of the phase separated domains. On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 4 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -2.0kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 6 shows that the mixing energy for the system was small for the temperature range studied. The graph indicated that an increase in temperature decreased the mixing energy upto 160 K. It indicates that mixing energy slowly increases with increase in temperature after 160 K upto 330 K and further increase in temperature with minimization of mixing energy. So, it is very much possible to mix the two components at high temperature with least mixing energy value. The homogeneous blend formation with polyvinyl alcohol as base might help formation of blend with high mechanical strength. This might have an application as packaging material and adsorbent.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly-1, 2-α-D-glucose to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair can have very good compatibility above 460 K. The coordination number was found to be 6.85 +/- 0.04. The maximum number of configurations with respect to energy level was found to be -2.0 kcal/mol. usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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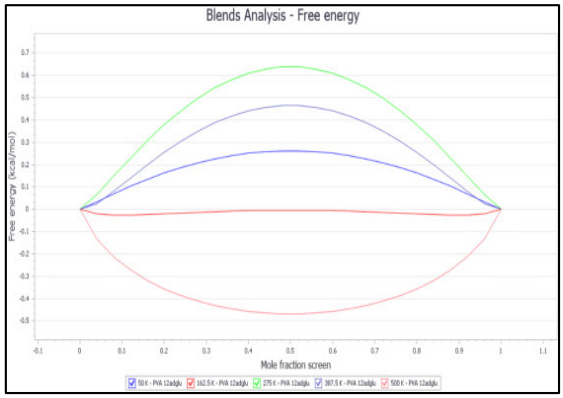

Figure 1. Free energy change with mole fraction of poly-1, 2-α-D-glucose at different temperatures

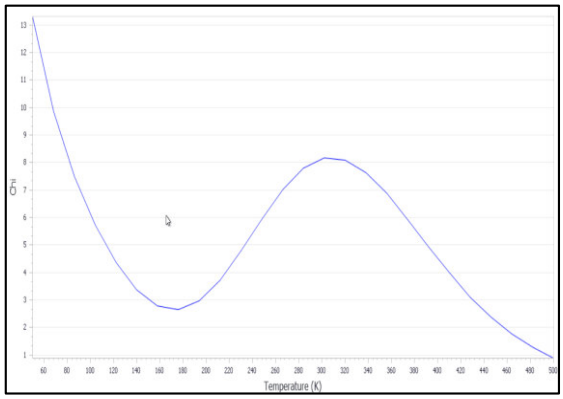

Figure 2. Change in χ (chi) value with temperature.

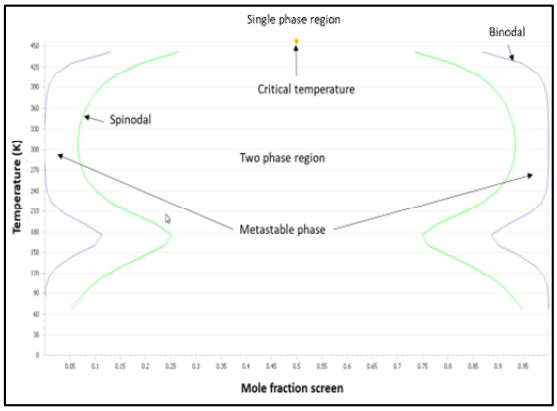

Figure 3. Phase diagram of the blend between polyvinyl alcohol and poly-1, 2-*α*-D-glucose.

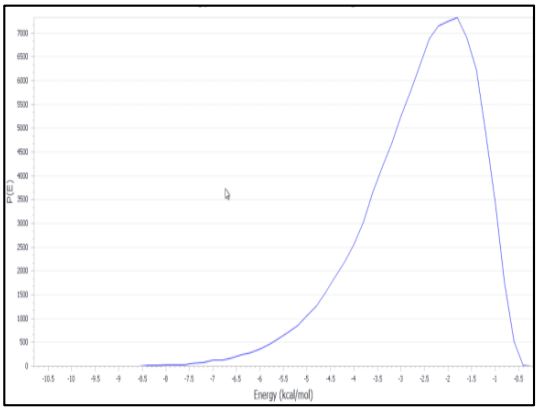

Figure 4. Energy distribution

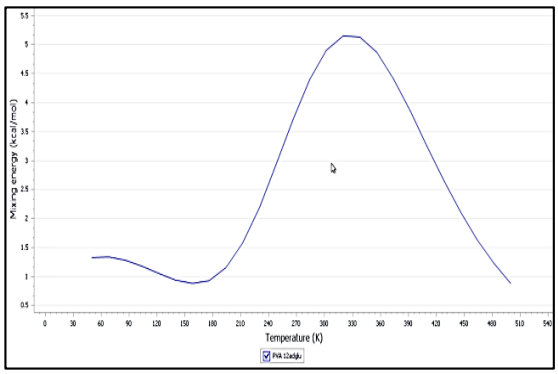

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyvinyl Alcohol and Poly-1, 2-α-D-Glucose Composite

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ABSTRACT

Polymerblends/composites are developed by varying the mass fraction of components to get anticipated properties. The desired property of a blend is its homogeneity, perhaps it may be heterogeneous. In this work, the in silicothermal and dielectric properties are explored taking polyvinyl alcohol and poly-1,2-α-D-glucose as components using Biovia material studio synthia analysis. The thermal and dielectric properties are exploredconcerning heat capacity, thermal conductivity, and dielectric constant. The results indicated that all those parameters decreased with anincrease in the mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money, and time.

Keywords: Synthia, in silico, polyvinyl alcohol, poly-1, 2-α-D-glucose, biovia material studio, thermal property, dielectric property

INTRODUCTION

Blends or composites are the physical combinations of more than one component where components do retain their identity in the mixture.The blend may be a homogenous or heterogeneous mixture. A single material cannot provide multiple anticipated properties. It is desirable to combine different components thereby improving the properties of the material. The development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus blending is a process that provides an easy pathwayto develop a new material by reducing the cost of development of products with preferred properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer. A composite/blend's characteristics differs from it's constituent components which are physically distinct from each other. Usually, a composite is a matrix in which strong and stiff reinforcement is distributed but made of soft and weaker components [1-3].The upgraded properties of composites are predominantly governed by

their microstructure and interaction between matrix and reinforcing materials in the inter-phase region [4, 5].Polymers coupled with carbon-based (graphene, carbon nano-tube) nano-materials [6] have drawn significant attention in recent years. Biodegradable polymers- natural fiber composites [7] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fireproof materials [8]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [9].

Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [10]. There are applications of composites in structural engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [11] were developed for the construction of bridges, light rail transit, mining, and tunneling, retaining walls, and other waterside buildings. All the above-mentioned examples relied on laboratory experiments. Usually, blends are prepared by trial and error method and this technique is a low cost and less time-consuming method. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [12]) has been used to identify compatible pairs.

Among the various polymers, polyvinyl alcohol (PVA) is a suitable material as it has high dielectric strength, easy film formation, adhesiveness, and whose properties can be controlled by dopant concentrations [13, 14]. The film-forming ability of PVA is widely used in the packaging industry to form strong polymeric films due to their high mechanical strength, environmental stability, and easy processability [15]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible, and easily soluble in water [16]. Researchers have found applications of glycopolymers (synthetic polymers containing pendant carbohydrate groups) in the separation and removal of toxins and bacteria, tumor cell recognition, and glucose-responsive insulin delivery [17]. It has been found that biopolymer blends possess good thermal stability [18].By adding glycopolymers (cellulose nanoscale fillers) in different polymers (polyvinyl alcohol or polylactic acid) we can generate nanocomposites resulting in mechanical reinforcement and alternation of other properties [19].This study is intended to identify the interaction of polyvinyl alcohol and poly-12-a-D-glucose to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and poly-1, 2-α-D-glucose were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work, the use of polyvinyl alcohol and poly-1, 2-α-D-glucoseaspotential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties.

Heat capacity: It is the amount of heatrequired to raise the temperature of one unit weight of a substance by 1°C without change of phase.Figure 1 shows that the heat capacity (Cp) of the composite decreases with increase in the mass fraction of vinyl alcohol.

Thermal conductivity: It indicates the correlation between heat flux per unit area and temperature gradient.It refers to the intrinsic ability of a material to transfer heat.Figure 2 shows that the thermal conductivity of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Dielectric constant: It is defined as the ratio of the electric permeability of the material to the electric permeability of free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant.Figure 3 shows that the dielectric constant of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly-1, 2-α-D-glucose to form a blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant.The results indicated that allthree parametersdecreased with an increase in the mass fraction of vinyl alcohol. Usually, components for a blend are identified experimentally. This in silico study will help determine the properties of a composite without performing laboratory experiments saving materials, money, and time.

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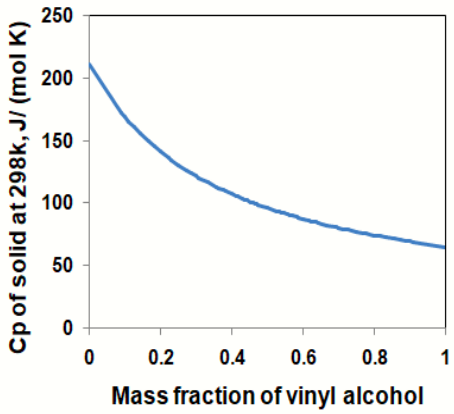

Figure 1. Change in heat capacity with mass fraction of vinyl alcohol

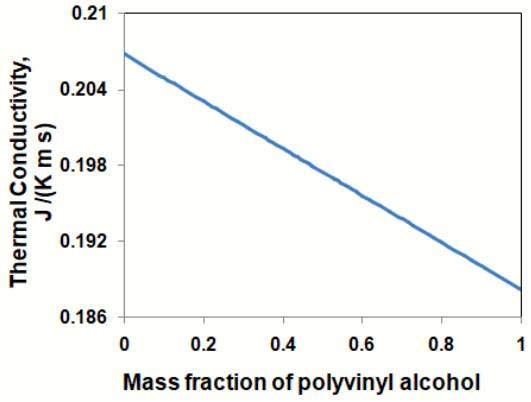

Figure 2. Change in thermal conductivity with the mass fraction of vinyl alcohol

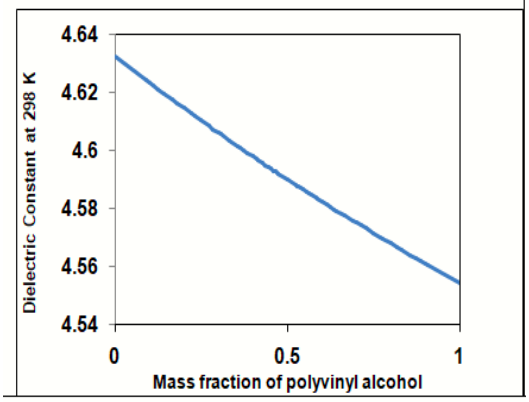

Figure 3. Change in dielectric constant with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyvinyl Alcohol and Poly-1, 2-α-D-Galactose Composite

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ABSTRACT

A blend is a combination of at least two components which gives superior properties than individual component. The heat capacity, thermal conductivity and dielectric constant of as-formed blend were studied using Biovia Material studio. The outcomes demonstrated that each one of those parameters decreased with increase in mass fraction of polyvinyl alcohol. That means heat capacity, thermal conductivity and dielectric constant of as-formed blend increased with increase in mass fraction of 1, 2-α-D-galactose. This study will help to determine pairs without doing experiments in laboratory sparing materials and time with low cost.

Keywords: In silico analysis; Dielectric properties; Thermal properties; Polyvinyl alcohol

INTRODUCTION

Blends or composites are materials containing more than one component. The components don't lose their character in the blend. They join and add to the property of the mix in this manner enhancing the quality of the material. Advancement of a solitary material with the ideal property includes significant research and time. A blend utilizes the advantages of different materials; mix them to get the wanted property. Thus a blend saves time to develop a new material thereby reducing the cost of improvement of products with required properties. Polymer blends can be made of at least two polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi-functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of

transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.

Among the different polymers, polyvinyl alcohol (PVA) is a auspicious material because of its high dielectric properties, easy film formation, adhesiveness and these properties can be influenced by dopant concentrations [8, 9]. The film forming ability of PVA is generally utilized in bundling industry to form strong polymeric films. It is a direct result of their high mechanical strength, environmental stability and easy processability [10]. Then again, PVA is hydrophilic, non-toxic, semi crystalline, easily soluble in water and biocompatible [11]. D-galactose has been used in combination with other materials in various applications in earlier literature [12]. Poly-1, 2-α-D-galactose has been demonstrated to be used in Curtius reaction. In this paper, the thermal and dielectric properties of blend of polyvinyl alcohol and poly-1, 2-α-D-galactose were analyzed at different mass fraction of vinyl alcohol using Discovery material studio which is new according to my knowledge.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and poly-1, 2-α-D-galactose were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly-1, 2-α-D-galactose as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties.

Heat capacity: It is the amount of heat required to raise the temperature of one unit weight of a substance by 1°C without change of phase. Figure 1 shows that the heat capacity (Cp) of the composite decreases linearly with increase in mass fraction of vinyl alcohol. Therefore we can say that the heat capacity (Cp) of the composite increases linearly with increase in mass fraction of 1, 2-α-D-galactose.

Thermal conductivity: It indicates the correlation between heat flux per unit area and temperature gradient. It refers to the intrinsic ability of a material to transfer heat. Figure 2 shows that the thermal conductivity of the composite decreases linearly with increase in mass fraction of vinyl alcohol. Therefore we can say that the thermal conductivity of the composite increases linearly with increase in mass fraction of 1, 2-α-D-galactose.

Dielectric constant: It is defined as the ratio of the electric permeability of the material to the electric permeability of free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant. Figure 3 shows that the dielectric constant of the composite decreases with increase in mass

fraction of vinyl alcohol. Therefore we can say that the thermal conductivity of the composite increases linearly with increase in mass fraction of 1, 2-α-D-galactose.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly-1, 2-α-D-galactose to form a blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The outcomes demonstrated that each one of those parameters decreased with increase in mass fraction of polyvinyl alcohol. That means heat capacity, thermal conductivity and dielectric constant of as-formed blend increased with increase in mass fraction of 1, 2-α-D-galactose. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without examining laboratory experiments that mean there is no use of any chemicals to analyze the above properties.

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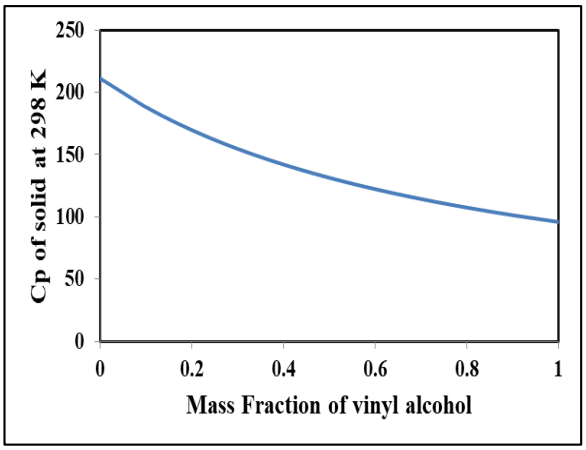

Figure 1. Change in heat capacity with mass fraction of vinyl alcohol

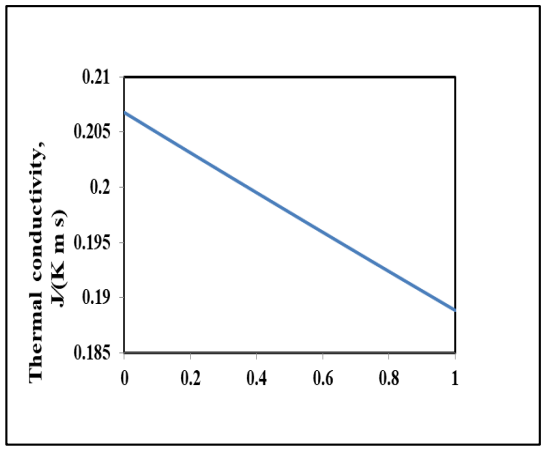

Figure 2. Change in thermal conductivity with mass fraction of vinyl alcohol

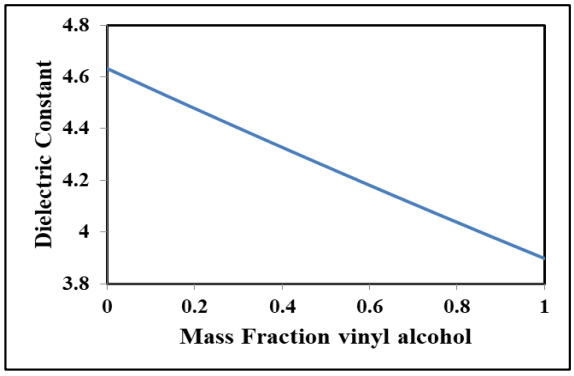

Figure 3. Change in dielectric constant with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Polyvinyl Alcohol Acid and Poly-1, 2-α-D-Galactose Compatibility in a Blend

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ABSTRACT

A blend is formed from the combination of two or more components. The compatibility of polyvinyl alcohol and poly-1, 2-α-D-galactose was studied to form a miscible blend using Biovia Materials Studio. The compatibility of the two components was demonstrated based on free energy of mixing, mixing energy and chi parameter. From the results, it was observed that the pair can have very good compatibility at low to high temperature without any phase separation. The coordination number was found to be 6.97 +/- 0.04. The highest number of configurations with respect to energy level was found to be -1.95 kcal/mol. This study will not only help to determine pairs without performing laboratory experiments but also less time consuming and low cost process.

Keywords: Blend; Biovia Material Studio; Compatibility; Polyvinyl alcohol; In silico analysis

INTRODUCTION

Blends or composites are formed with combination of more than one component where components do retain their identity in the mixture. As it is incredibly tough to seek out multiple properties during a single material, it's suggested to mix totally different component thereby enhancing the properties of the material. Development of one material with the required property involves important analysis and time. A blend utilizes the benefits of various materials; mix them to urge the required property. Therefore a blend saves time to develop a brand new material thereby reducing the price of development of products with desired properties. Polymer blends may be made of two or additional polymers, or fibers and polymer, or particles and polymer.

Nano material incorporated polymers paved the way to multi-functional materials. Polymers assisted with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been taken to enhance mechanical properties and water resistance. Further, the improved fire retardant/fire proof materials have been reported [3]. There are reports of inorganic additives in polypropylene; that

can enhance flame retardancy without increasing the weight [4]. Researchers have given attention on synthesis and production of lightweight composite materials having high strength necessary for improving fuel efficiency in the field of transportation [5]. There are various applications of composites in structural Engineering because of high strength to weight ratio and resistance to corrosion. Thus, glass fiber incorporated polymers; latex polymer cementations composites [6] were synthesized for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method and this technique is a low cost and less time consuming method. Thus, researchers have given attention on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs. Considering different polymers, polyvinyl alcohol (PVA) is a encouraging material because of its easy film formation, high dielectric strength, adhesiveness and its properties are often controlled by dopant concentrations [8, 9]. The film forming ability of PVA is wide employed in packaging trade to create sturdy compound films. It's as a result of their high mechanical strength, environmental stability and simple processability [10]. Further, PVA is non-toxic, hydrophilic, semi crystalline, biocompatible and easily soluble in water [11]. Scientist have found different applications of glycopolymers (synthetic polymers containing pendant carbohydrate groups) in the separation and removal of toxins and bacteria, tumor cell recognition and glucose-responsive insulin delivery [12]. It has been found that biopolymer blends possess good thermal stability [13].This study is intended to identify the interaction of polyvinyl alcohol and poly-1, 2-α-D-galactose to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: Polyvinyl alcohol and poly-1, 2-α-D-galactose was prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyvinyl alcohol was used as the base and poly-1, 2-α-D-galactose was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly-1, 2-α-D-galactose as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where ΔG_m = *Gibb's free energy of mixing*

ΔH_m = *Enthalpy of mixing*

ΔS_m = *Entropy of mixing*

T = *Absolute temperature*

The value of $T\Delta S_m$ is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpy contribution, i.e.,

$$\Delta H_m < T\Delta S_m \quad (2)$$

Figure 1 shows that the free energy involved in mixing is always negative or less than zero for the temperatures studied. The free energy decreases with increase in temperature (up to 275 K) as evident from Eq. 1 and then free energy increases with increase in temperature (up to 500 K). The results indicated that the blend will absolutely lead to a homogeneous mixture for the temperature range studied (50 to 500 K). The trend shows a very good compatibility between polyvinyl alcohol and poly-1, 2-α-D-galactose with negative value of mixing energy, which may lead to form a perfect blend with significantly less effort.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similar components may lead to a high positive value of χ (chi).

Figure 2 shows that the χ value is very small or negative for the temperature range studied (50 to 500 K) indicating very good mixing. The χ value increased with an increase in temperature at various temperatures ranges (50 K to 500 K). There is a very good possibility of homogeneous mixing with such small value of χ which agrees with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size. In this study the coordination number was found to be 6.97 +/- 0.04.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 4 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -1.95 kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 5 shows that the mixing energy for the system was small for the temperature range studied. The graph indicated that an increase in temperature results the increase in mixing energy. It also shows that mixing energy gradually increases with increase in temperature with varying the temperature from 50 K to 500 K. So, it is very much possible to mix the two components at any feasible temperature with least mixing energy value.

The formation of non homogeneous blend with polyvinyl alcohol as base might help formation of blend with high mechanical strength. This might have an application as packaging material and adsorbent.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly-1, 2-α-D-galactose to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair can have very good compatibility at different ranges of temperature. The coordination number was found to be 6.97 +/- 0.04. The maximum number of configurations with respect to energy level was found to be -1.95 kcal/mol. usually components for a blend are identified experimentally. This in silico study will help to determine components of a blend without performing laboratory experiments saving materials, money and time.

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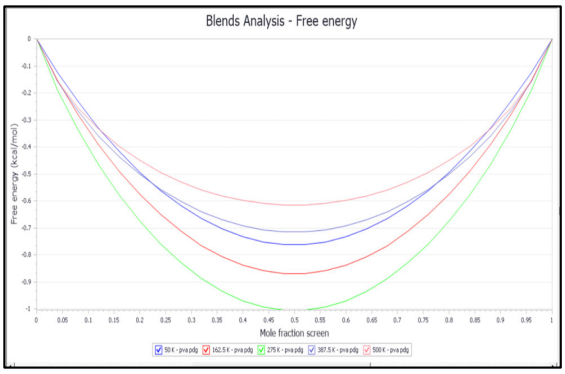

Figure 1. Free energy change with mole fraction of poly-1, 2-α-D-galactose at different temperatures

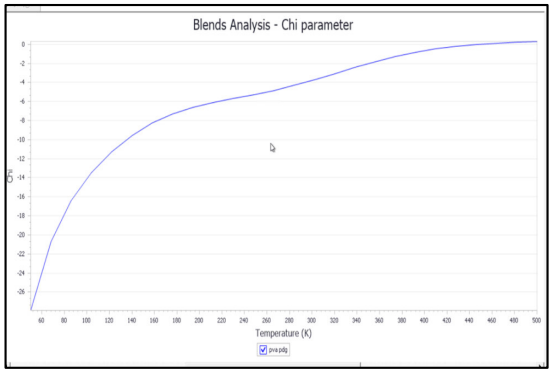

Figure 2. Change in χ (chi) value with temperature

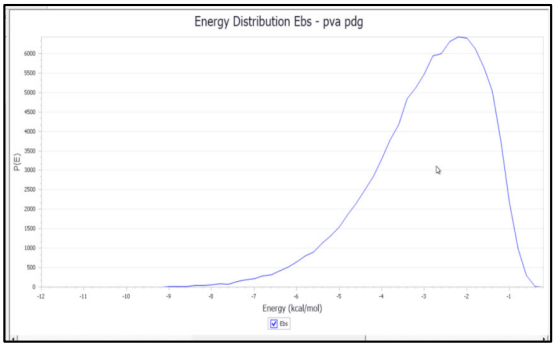

Figure 3. Energy distribution

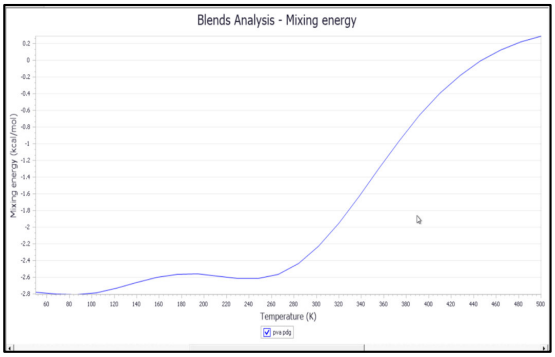

Figure 4. Mixing energy

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RESEARCH ARTICLE

In silico Blend Compatibility Investigation of Poly (Biphenyl Dimethyl Carbonate) and Polydimethyl Siloxane

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ABSTRACT

Polymeric blend having two or more components is the easiest and low cost way to generate hybrid polymer with improved properties. Strong molecular interaction in homogeneous blend is the key to enhance the physical and chemical properties of polymers. In this manuscript, we have tried to explore the compatibility of poly (biphenyl dimethyl carbonate) and polydimethylsiloxaneto form a miscible blend using Biovia Materials Studio. The blending compatibility of these two polymers was studied based on free energy of mixing, phase diagram, chi parameter, and mixing energy.The obtained results depicted that the compatibility between these two polymers only possible in the temperature range of 270 K to 300 K. However, higher and lower temperature may lead the phase separation between these two polymers. But at very higher temperature (1080 K) single phase may exist as revealed from the phase diagram. The coordination number wasfound to be 3.14 +/- 0.02. The highest number of configurations with respect to energy level was found to be -2.5 kcal/mol. This study may help in determining the optimal composition of pairs and temperature for the preparation of homogeneous blend without performing laboratory experiments and therefore, saving materials, money and time.

Keywords: Blend; *In silico* analysis Poly (biphenyl dimethyl carbonate) and poly dimethyl siloxane

INTRODUCTION

The recent age is basically dealing with the improvement of existing one in all dimensions starting from the industrial to biomedical sectors. Polymers are simply long chain macromolecules with man-made or natural origins. It shows a repetition in their distinguished structural units and well known for their ability to be utilized in daily needs [1]. The frequently-used method of modifying the properties of polymers is their blending with other natural or synthetic polymers and it leads to the improvement in various properties like thermal [2], mechanical [3] and electrical properties [4]. The preparation of miscible blends allows most strongly changing the properties of

polymers; however, there are not so many pairs of polymers forming such blends [5]. In majority of cases, polymers form miscible blends only in the case of a low content of one of them , or they are low molecular weight or due to the addition of a compatibilizer [6]. From the thermodynamic point of view, miscibility of a blend depends upon the decrease of Gibbs free energy of mixing and related to change in entropy and enthalpy. Therefore, the investigation of mixing compatibility or miscibility of a pair of blends is the crucial parameter to prepare hybrid polymers with improved properties. Moreover, with the recent scenario, hybrid polymers are widely used with nanostructural filler (carbon nanotube, nanoclay, graphene, etc.) to deliver excellent properties such as electrical or semiconducting [7], thermal [8] and mechanical properties [9]. Among different polymers, poly (biphenyl dimethyl carbonate) (PC) is a widely used engineering plastics because of its physical and chemical properties like ductility, good thermal stability, excellent transparency, and high mechanical strength [10]. As a resultof these excellent properties, PC has been largely employed in electronic and electronic appliances along with automotive industry, having an annual production of 6 million tons. Recent report by Behboudiet. al. [11] shows thatPC is blended withpolyvinyl chloride (PVC)to preparethe ultrafiltration membrane for water purification. On the other hand, PC is also blended with poly (vinylidene fluoride) (PVDF) to prepare mechanically strong multicomponent nanocomposites with nanostructural reinforcement of graphenenanoplates, carbon nanotube, and organically modified montmorillonite [12].

In another recent report Wen et al. reinforced the graphene plates into blend of polybutyleneterethalateand polycarbonate [13] to obtain electrical and thermal conductive materials. The unique material, formed from the blend of PC with polystyrene is also reported to sense organic vapours with incorporation of multiwalled carbon nanotubes (MWCNTs) [14]. Polycarbonate blendedpolysulfone material is recently observed to have improved thermal and mechanical properties.[15]Therefore,investigationof blending compatibility of polycarbonate with other polymer is the urgent need of current research to develop advanced functional materials.All the above mentioned examples relied on laboratory experiments. Usually, preparation of homogeneous blend in wet-lab condition requires huge time and wastage of materials which can be minimized by in-silico approach through material studio [16] of "Biovia" software. In present context, we are focusing to optimize the homogeneous blend composition of polybiphrnyldimethylcarbonate (PC) with polydimethylsiloxane (PDMS). It is a polymeric organosilicon compound, particularly known for its unusual rheological behaviors. Moreover it is optically clear, non-toxic and non-flammable. Polydimethylsiloxane (PDMS) shows wide applications like contact lenses, medical devices and preparing elastomer materials. It is also used in making of lubricants and heat-resistant tiles. Recently, Adreeset. al. [17] prepared the PDMS based blend membranes with polyvinyl chloride-co-vinyl acetate (PVCA) for CO_2seperation. Polydimethylsiloxane is also used in biomedical application like maxillofacial prosthetics, artificial blood vessels and articular cartilage replacement, when it is blended with poly ether (ether) ketone (PEEK) [18]. Therefore, the present in-silico approach of blend analysis between polybiphenyldimethyl carbonate (PC) and polydimethylsiloxane (PDMS) may be utilized to optimize the composition to fabricate desirable functional materials with some improved physical and chemical properties.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for this blend analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: Poly (biphenyl dimethyl carbonate) and polydimethylsiloxane were prepared using the build menu of theMaterials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. polybiphenyl dimethyl carbonate was used as the base and polydimethyl siloxanewas used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed in order to gain knowledge regarding the compatibility of the components to form a blend.

RESULTS AND DISCUSSION

In this investigation, we have used poly (biphenyl dimethylcarbonate) (PC) and polydimethylsiloxaneas potential components of a blend and it was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$\Delta G_m - \Delta H_m - T\Delta S_m$ (1)

Where, $\Delta G_m = Gibb\ s\ free\ energy\ of\ mixing$

$\Delta H_m = Enthalpy\ of\ mixing$

$\Delta S_m = Entropy\ of\ mixing$

$T = Absolute\ temperature$

The value of $T\Delta S_m$ is always positive in case of a blend, since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$\Delta H_m < T\Delta S_m$ (2)

Figure 1, shows that the free energy involved in mixing is initially positive and goes on decreasing with increase of temperature upto275 K, after that starts increasing and approaches to a positive value (~2.7 Kcal/mole) at a temperature of 500 K. The initial decrement in the free energy with increase in temperature upto 275 K from positive value to slight negative value is observed. Small negative values at 275 Kindicates that the blend with all compositions of PC and PDS have a homogeneous composition at temperature 275K. This offers a very good compatibility between these two polymers, i.e. polybiphenyl dimethyl carbonate (PC) and polydimethylsiloxane and therefore, showing the best way to prepare the hybrid polymer film. But as we increase the temperature above (~300K), homogeneity in the polymer blend is disturbed and a immiscible pair is obtained instead of a perfect blend.

Phase diagram: Fig. 2 represents the phase diagram of the blend having poly (biphenyl dimethyl carbonate) (PC) and polydimethylsiloxane (PDMS) in their composition. Phase diagram is particularly helpful in predicting the different region of varying miscibility in connection to the temperature and composition. In present figure 1080 K shows the upper critical solution temperature (UCST) above which single phase miscible region is observed. Fragmented metastable region is observed in between bimodal (blue lines) and spinodal lines (green lines). The region of phase separation is underlined by spinodal, whereas, bimodal separates the single-phase and meta-stable region.When the system enters from single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e, slow nucleation followed by growth of the phase separated domains. On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similar components may lead to a high positive value of χ (chi).Figure 2 shows that the blend of PC and PDMS has basically depicted the positive values of χ (chi) within a temperature range of 50 K to 500 K. It confers the de-mixing of these two polymeric components due to mis-matching of their cohesive energy within the whole temperature range. But, interestingly, near the temperature of

270-300 K, it approaches to value with showing the possibility of mixing. Above this temperature (> 300 K), χ of this blending again approaches to a high positive value andtherefore, represents a state of phase separation. However, poly (biphenyldimethylcarbonate) (PC) and polydimethylsiloxane (PDMS) are well mixed to form a homogeneous blend only in the temperature range of 270-300 K and the data is well supported from the free energy of mixing of the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It is assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size. In this study the coordination number was found to be 3.10 +/- 0.02.

Energy Distribution for Blend: Fig.4 shows the variation of population of different energy levels associated with pair having different configuration and orientation. It shows that the distribution shows a broad curve with long tail. Maximum population is centered around -2.5 Kcal/mol energy and distribution around this value is asymmetric in nature. As expected majority of pair configuration lies on the low energy value to attain a stable state of miscibility.

Mixing Energy: A small value of mixing is generally allows the polymeric components to mix well to get the homogenous blend. Thus, the temperature at which the mixing energy is low may be suitable for mixing. Figure 5 shows that the mixing energy for the system was small for the temperature range of 270-300K, while it shows the higher values for other temperature domain. Hence, the mixing of these two polymeric component is only possible in the region of 270-300K.

CONCLUSION

The possibility of use of poly (biphenyl dimethyl carbonate) and polydimethyl siloxane and to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair can have the compatibility at 270-300K; beyond that phase separation may results. The coordination number was found to be 3.14 +/- 0.02. The maximum number of configurations with respect to energy level was found to be -2.5 kcal/mol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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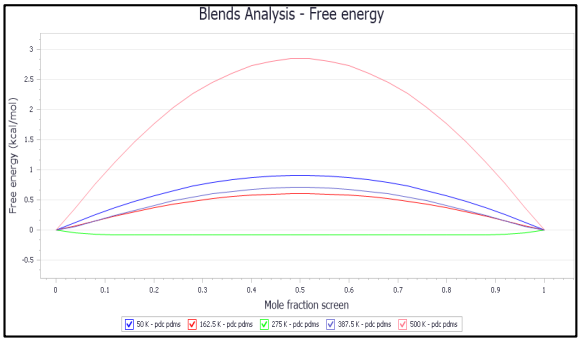

Figure 1. Free energy change with mole fraction of polydimethylsiloxaneat different temperatures

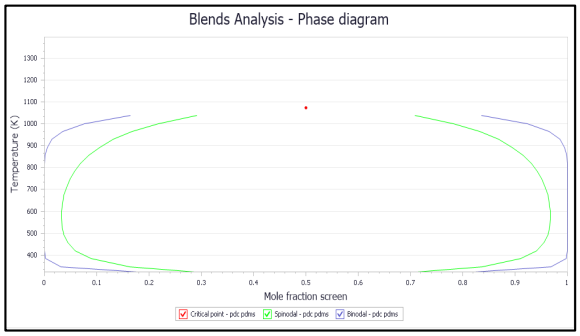

Figure 2. Phase diagram of the blend

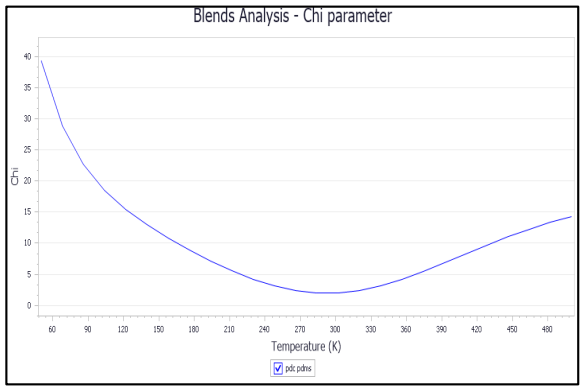

Figure 3. Change in χ (chi) value with temperature

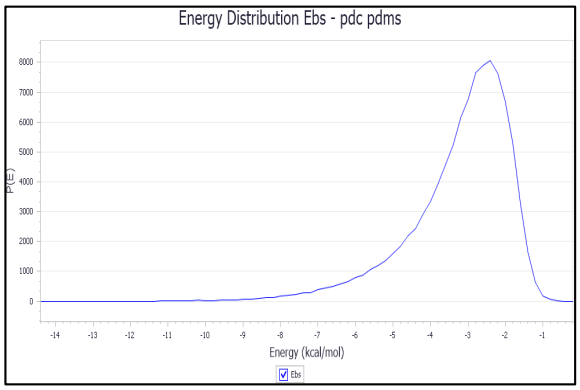

Figure 4. Energy distribution

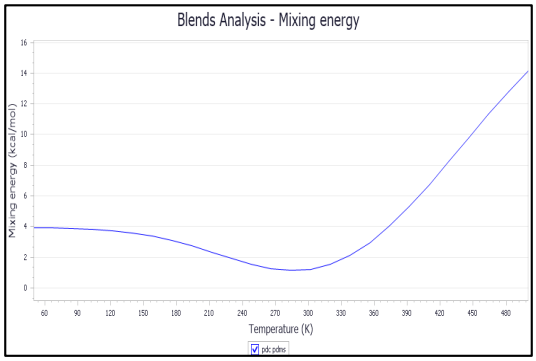

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyacrylic Acid and Poly-1,3-α-D-Galactose compatibility in a Blend

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ABSTRACT

A blend is always a composition of two or more components and it is desirable to have homogeneityin a blend. In this paper, we have tried to explore the compatibility of polyacrylic acid andpoly-1,3-α-D-Galactoseto form a miscible blend using Biovia Materials Studio. The compatibility of the two components was studied based on free energy of mixing, chi parameter, and mixing energy. The results indicated that the pair havea very good compatibility with a positive value of mixing energy within temperature range considered. The coordination number was found to be 7.22 +/- 0.05. The highest number of configurations with respect to energy level was found to be -2.2 kcal/mol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: In silico analysis, Blend, Biovia Materials Studio, polyacrylic acid, poly-1,3-α-D-Galactose.

INTRODUCTION

Blends or composites are materials containing more than one component. The components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisableto combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance

flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs. Acrylic polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects etc. [8], bone repair [9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc.[10]. Polyacrylic acid is a polyelectrolyte soluble in aqueous media at neutral pH It is used for preparing hydrogels. It is not toxic and does not cause irritation [11]. Researchers have found applications of glycopolymers (synthetic polymers containing pendant carbohydrate groups) in the separation and removal of toxins and bacteria, tumor cell recognition and glucose-responsive insulin delivery [12].It has been found that biopolymer blends possess good thermal stability [13].This study is intended to identify the interaction of polyacrylic acid and poly-1,3-α-D-Galactoseto form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: Polyacrylic acid and poly-1,3-α-D-Galactosewere prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyacrylic acid was used as the base and poly-1,3-α-D-Galactosewas used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acid and poly-1,3-α-D-Galactoseaspotential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where $\Delta G_m = Gibbs\,free\,energy\,of\,mixing$

$\Delta H_m = Enthalpy\,of\,mixing$

$\Delta S_m = Entropy\,of\,mixing$

$T = Absolute\,temperature$

The value of $T\Delta S_m$is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_malways depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$$\Delta H_m < T\Delta S_m \quad (2)$$

Figure 1 shows that the free energy involved in mixing is always positive for the temperatures studied. The free energy decreases with increase in temperature for the system under study as is evident from Eq 1. The results

indicated that the blend will not supportthe formation of a homogeneous mixture for the temperature range studied (50 to 500 K). The trend shows the mismatching between polyacrylic acid and poly-1,3-α-D-Galactosewithpositive value of mixing energy and thus getting a perfect blend within the temperature range is somewhat intricate.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymershaving small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains.Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similarcomponentsmaylead to a high positive value of χ (chi).

Figure 2 shows that the χ value is positive within the temperature range under study (50K to 500K) indicating very poor mixing. The χ value decreasedwith increase in temperature constantly.Thus there is a possibility of getting homogeneous mixturebetween the polymers taken at a very high temperature.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size.In this study the coordination number was found to be7.22 +/- 0.05.

Energy Distribution for Blend: The generation of different orientations using the pairsmethod may lead to configurations of varying energy levels. Figure 4 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreasedsignificantly. The maximum frequency was observed for the energy level of around -2.2kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing.The mixing energy for the system is positive within the temperature range studied as shown in the Figure 5. The graph indicated that an increase in temperatureincreased the mixing energy consistently and exponentially from 25kcal/mol to 35kcal/mol for a temperature increment of 50K to 500K.So,the mixing of the two components under study needs very high energy within the temperature range under study.

CONCLUSION

The possibility of use of polyacrylic acid and poly-1,3-α-D-Galactoseto form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the components within the pair are notcompatiblewithin the temperature range 50K to 500K. The coordination number was found to be 7.22 +/- 0.05. The maximum number of configurations with respect to energy level was found to be -2.2 kcal/mol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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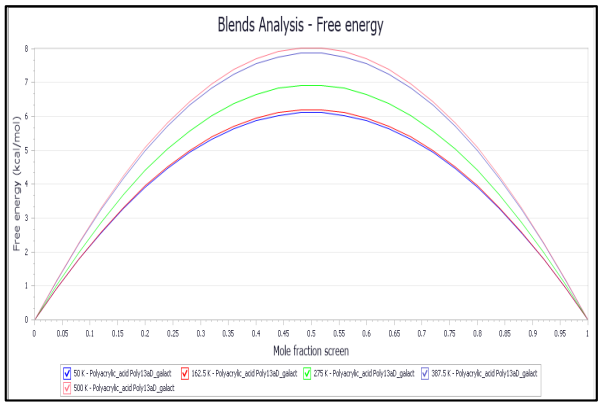

Figure 1. Free energy change with mole fraction of Galact 13adat different temperatures

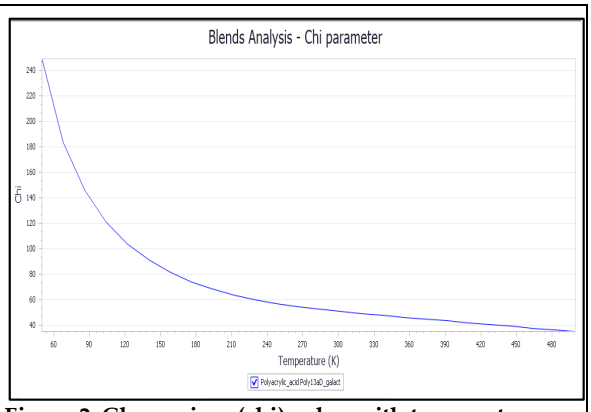

Figure 2. Change in χ (chi) value with temperature

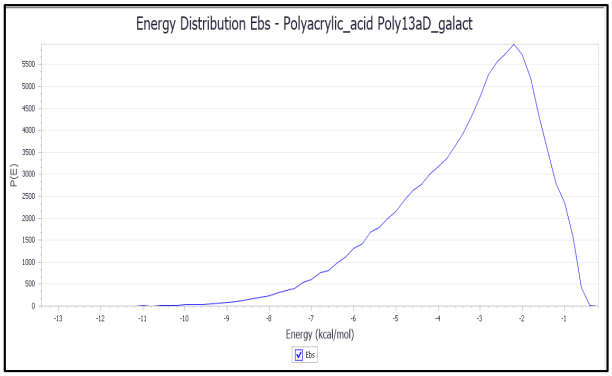

Figure 3. Energy distribution

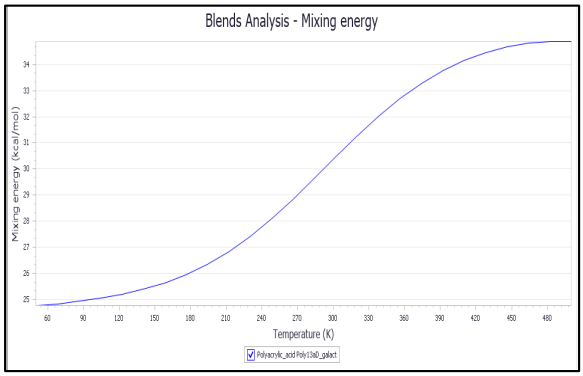

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyacrylic Acid and Polyacrylochloride Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all those parameters increased with increase in mass fraction of acrylic acid. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Polyacrylic, Polyacrylochloride composite

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were

developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs. A broad variety of applications of acrylic polymers in dental surgery as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects etc. [8], bone repair [9], dispersing agent, super absorbent polymer, ion-exchange resin, etc.[10].

Polyacrylic acid is a polyelectrolyte soluble in aqueous media at neutral pH.It is used for preparing hydrogels. It is not toxic and does not cause irritation [11]. Researchers have used polyacrylochloride in combination with other materials to act as adsorbent [12]. Polyacrylochloride have been reported to be used in Curtius reaction. This study is intended to identify the interaction of polyacrylic acid and polyacrylochloride to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systems of France) was utilized for analysis. The software applies machine learning schemes and standard algorithms to forecast the standard of interactivity.

Methodology: The structures of polyacrylic acid and polyacrylochloride were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyacrylic acid on the mechanical properties of the composite

RESULTS AND DISCUSSION

In this work the use of polyacrylic acid and polyacrylochloride as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia utilizes pre-arranged correlations (advanced quantitative structure-property relationships) to assess a broad range of polymer applications. Group additive methods were utilized for several years to forecast the applications of polymers as well as tiny molecules. These processes are very rapid and easy to utilize. In Consequence, they are of biggest usefulness when a very fast guessing of a property is needed without a thorough knowledge of the atomistic interactions that give rise to it. However, the main limitations of this process are their dependence on a database of group contributions. So, if a polymer carries a group for which the group contribution cannot be evaluated, then the property of that polymer cannot be estimated. To overcome this shortcoming, the process executed in Synthia utilizes topological knowledge about polymers in the anticipating correlations. The correlations indices obtained from graph theory are applied. Thus, no database of group contributions is needed and properties may be forecasted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Heat capacity: It is the amount of warmth needed to rise the temperature of one unit weight of a substance by 1°C without variation of phase. Figure 1 shows that the heat capacity (Cp) of the composite rises linearly with rise in mass fraction of acrylic acid.

Thermal conductivity: It indicates the correlation between heat flux per unit area and temperature gradient. It refers to the intrinsic ability of a material to transfer heat. Figure 2 shows that the thermal conductivity of the composite rises linearly with rise in mass fraction of acrylic acid.

Dielectric constant: It is determined as the fraction of the electric permeability of the material to the electric permeability of free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant. Figure 3 shows that the dielectric constant of the composite increases with rise in mass fraction of acrylic acid.

CONCLUSION

The possibility of use of polyacrylic acid and polyacrylochloride to form a blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all the three parameters increased with increase in mass fraction of acrylic acid. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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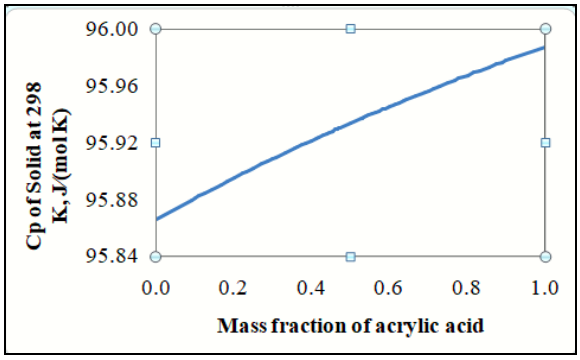

Figure 1. Change in heat capacity with mass fraction of acrylic acid

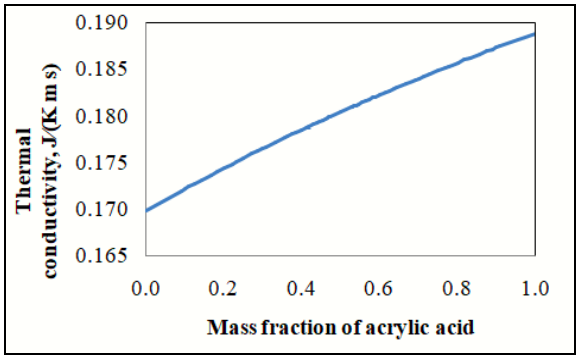

Figure 2. Change in thermal conductivity with mass fraction of acrylic acid

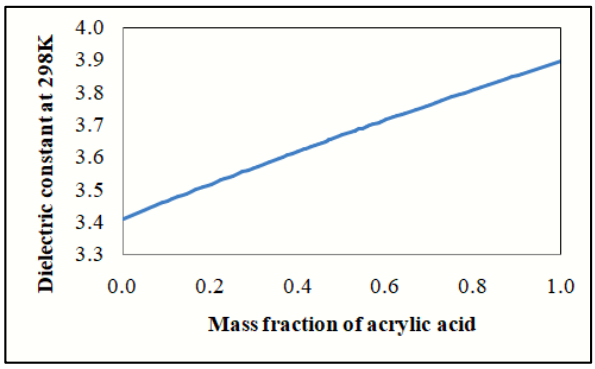

Figure 3. Change in dielectric constant with mass fraction of acrylic acid

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyacrylic Acid and Polyurea Composite

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ABSTRACT

A blend is a combination of more than one component or constituents. The desired property of a blend is its homogeneity. The composition of polyacrylic acid and polyurea to provide desired mechanical properties of the blend was explored using Biovia Material Studio. The composition of the blend was analyzed concerning permeability properties.The molar volume increased and density decreased with an increase in acrylic acid fraction. The permeability properties of the composite were studied based on the permeability of oxygen, nitrogen, and carbon dioxide. The results indicated that the permeability for all the gases has exponential growth from 0.8 to 1-mole fraction of acrylic acid. This study will help determine components of a blend without performing laboratory experiments saving materials, money, and time.

Keywords: polyacrylic acid, polyurea, in silico, permeability

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. The development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.Nanomaterial modified polymers paved the way for multifunctional materials. Polymers coupled with carbon-based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fireproof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of

lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were developed for the construction of bridges, light rail transit, mining and tunneling, retaining walls, and other waterside buildings. All the above-mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time, and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs.Acrylic polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects, etc. [8], bone repair [9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc. [10]. Polyacrylic acid is a polyelectrolyte soluble in aqueous media at neutral pH It is used for preparing hydrogels. It is not toxic and does not irritate [11]. This study is intended to identify the interaction of polyacrylic acid and polyurea to form blends.Polyurea is a type of elastomer that is derived from the reaction product of an isocyanate component and a synthetic resin blend component through step-growth polymerization. The isocyanate can be aromatic or aliphatic in nature. It can be monomer, polymer, or any variant reaction of isocyanates, quasi-prepolymer or a prepolymer. The prepolymer or quasi-prepolymer can be made of an amine-terminated polymer resin, or a hydroxyl-terminated polymer resin [12].

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and polyacrylochloride were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of the weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acid and poly urea as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar Volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite increases with an increase in mass fraction of acrylic acid.

Density: Increase in density indicates a decrease in porosity. A higher porosity will enhance the surface area making it suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite decreases with an increase in mass fraction of acrylic acid.

Permeability of Gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium.Lower permeability indicates a longer time lag for the gas to pass through the membrane. Figure 3 show that the permeability of oxygenthrough the composite has exponential growth from 0.8 to 1-mole fraction of acrylic acid.

Figure 4 show that the permeability of nitrogenthrough the composite has exponential growth during 0.8 to 1-mole fraction of acrylic acid. Figure 5 show that the permeability of carbon dioxide through the composite has exponential growth from 0.8 to 1-mole fraction of acrylic acid.

CONCLUSION

The possibility of the use of polyacrylic acid and polyureato form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed concerningpermeability properties.The molar volume increased and density decreased with an increase in acrylic acid fraction. The permeability properties of the composite were studied based on the permeability of oxygen, nitrogen, and carbon dioxide. The results indicated that the permeabilityfor all the gases has exponential growth from 0.8 to 1-mole fraction of acrylic acid.Usually components for blends are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money, and time.

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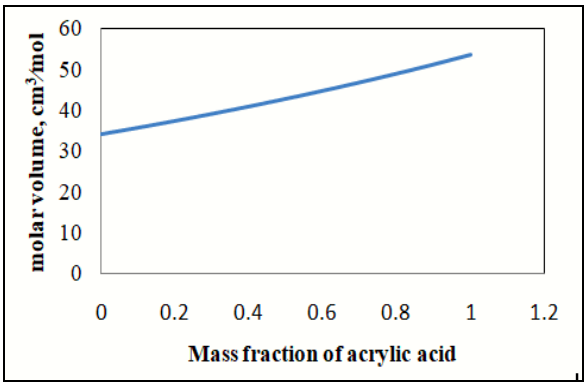

Figure1. Change in molar volume with mass fraction of acrylic acid

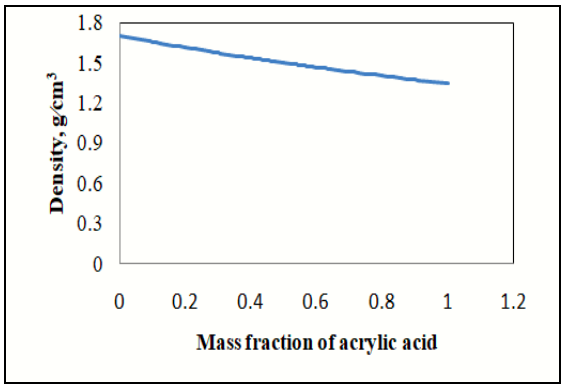

Figure 2. Change in density with the mass fraction of acrylic acid

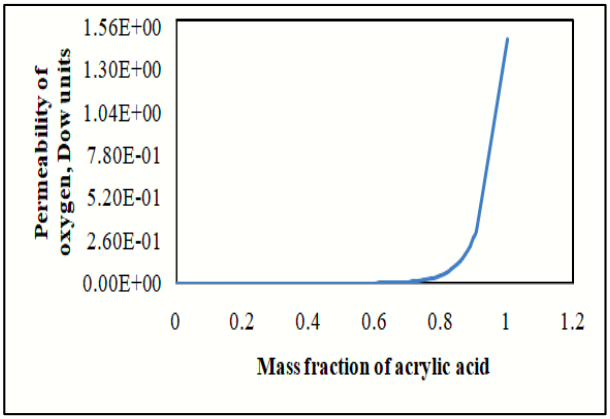

Figure3. Change in permeability f oxygen with the mass fraction of acrylic acid

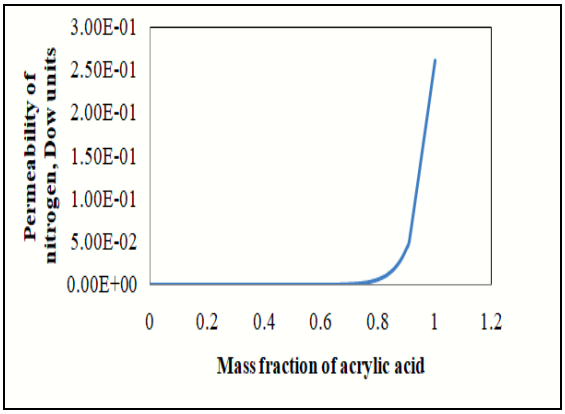

Figure 4. Change in permeability of nitrogen with the mass fraction of acrylic acid.

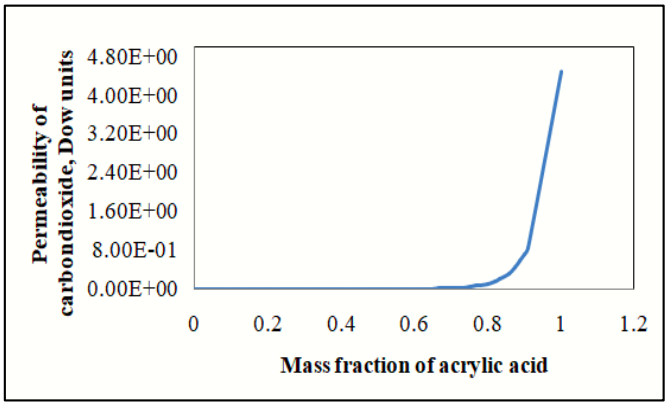

Figure5. Change in permeability of carbon dioxide with the mass fraction of acrylic acid.

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyvinyl Alcohol and Polyether sulfone Composite

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ABSTRACT

A blend is a combination of more than one component or constituents. The desired property of a blend is its homogeneity. The composition of polyvinyl alcohol and polyethersulfone to provide desired mechanical properties of the blend was explored using Biovia Material Studio. The composition of the blend was analyzed concerning permeability properties.The molar volume and density decreased with an increase in polyvinyl alcoholfraction. The permeability properties of the composite were studied based on the permeability of oxygen, nitrogen, and carbon dioxide. The results showed that the permeability for all the gases decreased withan increase in mass fraction of polyvinyl alcohol. This study will help determine components of a blend without performing laboratory experiments saving materials, money, and time.

Keywords: polyvinyl alcohol, polyethersulfone, in silico, permeability

INTRODUCTION

The blend may be a homogenous or heterogeneous mixture. Blends or composites are the physical combinations of more than one component where components do retain their identity in the mixture. A single material cannot provide multiple anticipated properties. It is desirable to combine different components thereby improving the properties of the material. The development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus blending is a process that provides an easy pathway to develop a new material by reducing the cost of development of products with preferred properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer. Polymers coupled with carbon-based (graphene, carbon nano-tube) nano-materials [1] have drawn significant attention in recent years. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fireproof materials [2]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without

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Usually, blends are prepared by trial and error method and this technique is a low cost and less time-consuming method. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs. Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness, and whose properties can be controlled by dopant concentrations [8, 9]. The film-forming ability of PVA is widely used in the packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability, and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible, and easily soluble in water [11].

Polyethersulfone (PES) is one of the most important engineering polymeric materials. This polymer is extensively used in membrane separation devices, such as microfiltration and ultra filtration (UF) process in the fields of food, plasma separator, biomedicine, hemodialysis, and water purification, etc.[12-15]. Besides, it displays exceptional thermal, oxidative, and hydrolytic stability as well as good mechanical and film-forming properties. It has been reported that blending PES with other polymers has addressed the surface physical and chemical properties concerning improved membrane properties, modifications of the pore structure, etc. [16]. This study is intended to identify the interaction of polyvinyl alcohol and poly(ether sulfone) to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and polyacrylochloridechloride were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of the weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

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Molar Volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite decreases with an increase in mass fraction of polyvinyl alcohol.

Density: Increase in density indicates a decrease in porosity. A higher porosity will enhance the surface area making it suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite decreases with an increase in mass fraction of polyvinyl alcohol.

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Figure 4 shows that the permeability of nitrogenthrough the composite decreases with an increase in mass fraction of polyvinyl alcohol. Figure 5 shows that the permeability of carbon dioxide through the composite decreases with an increase in mass fraction of polyvinyl alcohol.

CONCLUSION

The possibility of the use ofpolyvinyl alcohol acid and polyethersulfone to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed concerningpermeability properties.The molar volume and density decreased with an increase in polyvinyl alcoholfraction. The permeability properties of the composite were studied based on the permeability of oxygen, nitrogen, and carbon dioxide. The results showed that the permeability for all the gases decreased with an increase in mass fraction of polyvinyl alcohol.Usually components for blends are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money, and time

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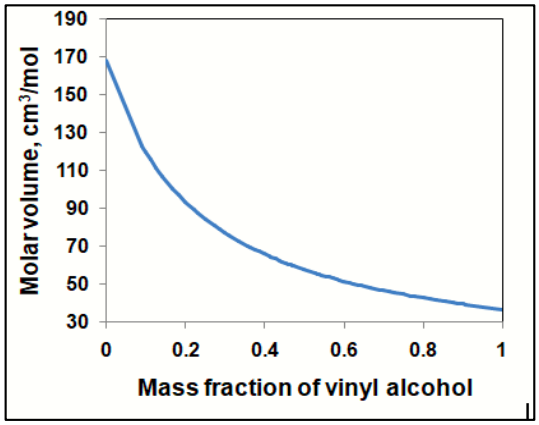

Figure1. Change in molar volume with the mass fraction of vinyl alcohol.

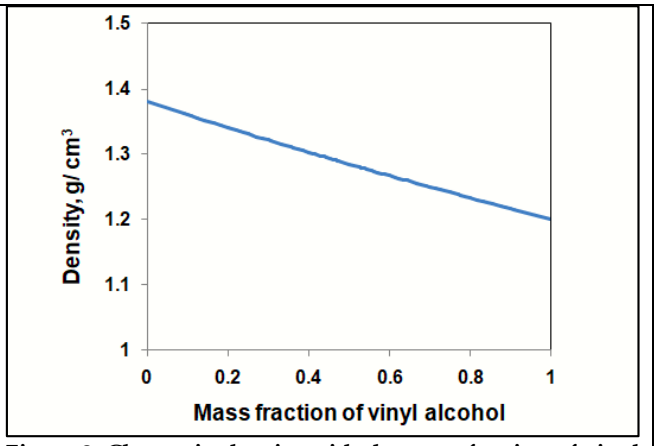

Figure 2. Change in density with the mass fraction of vinyl alcohol.

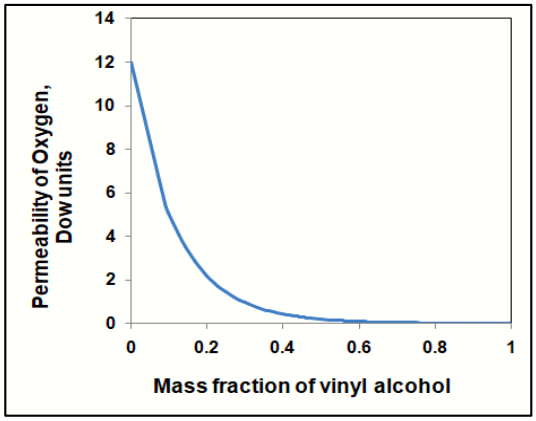

Figure3. Change in permeability of oxygen with the mass fraction of vinyl alcohol

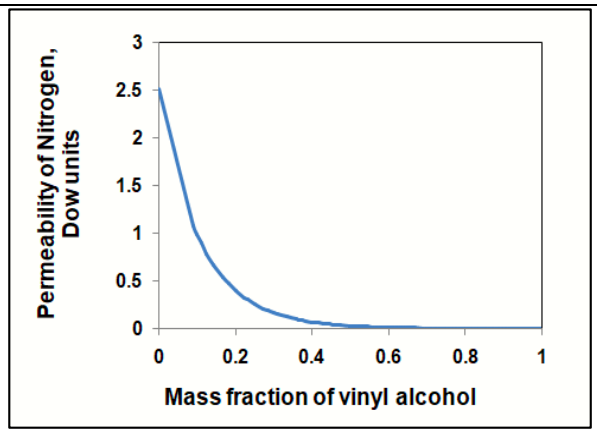

Figure 4. Change in permeability of nitrogen with the mass fraction of acrylic acid.

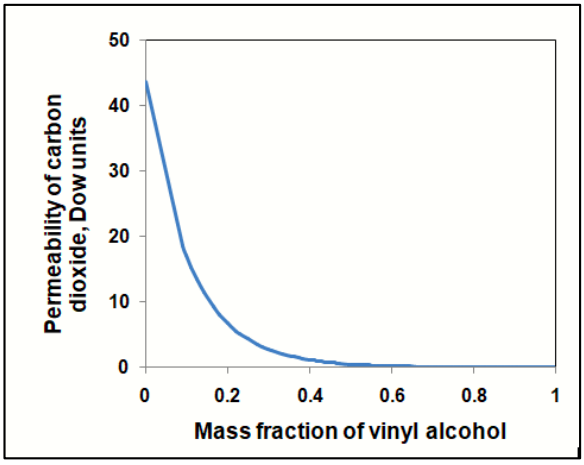

Figure 5. Change in permeability of carbon dioxide with the mass fraction of acrylic acid.

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RESEARCH ARTICLE

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ABSTRACT

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Keywords: mechanical, in silico,polyvinyl alcohol, polyethersulfone

INTRODUCTION

The blend may be a homogenous or heterogeneous mixture. Blends or composites are the physical combinations of more than one component where components do retain their identity in the mixture. A single material cannot provide multiple anticipated properties. It is desirable to combine different components thereby improving the properties of the material. The development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus blending is a process that provides an easy pathway to develop a new material by reducing the cost of development of products with preferred properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer. Polymers coupled with carbon-based (graphene, carbon nano-tube) nano-materials [1] have drawn significant attention in recent years. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fireproof materials [2]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4].

Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for the construction of bridges, light rail transit, mining and tunneling, retaining walls, and other waterside buildings. All the above-mentioned examples relied on laboratory experiments.

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Polyethersulfone (PES) is one of the most important engineering polymeric materials. This polymer is extensively used in membrane separation devices, such as microfiltration and ultrafiltration (UF) process in the fields of food, plasma separator, biomedicine, hemodialysis, and water purification, etc.[12-15]. Besides, it displays exceptional thermal, oxidative, and hydrolytic stability as well as good mechanical and film-forming properties. It has been reported that blending PES with other polymers has addressed the surface physical and chemical properties concerning improved membrane properties, modifications of the pore structure, etc. [16]. This study is intended to identify the interaction of polyvinyl alcohol and poly(ether sulfone) to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and polyacrylochloride were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of the weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcoholand polyether sulfone as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Bulk Modulus: Bulk modulus is the measure of the decrease in volume with an increase in pressure. Figure 1 shows that the bulk modulus of the composites increases with an increase in mass fraction of polyvinyl alcohol.

Shear Modulus: It is defined as the ratio of shear stress and shear strain. It shows the response of the composite to shear deformation. Figure 2 shows that the shear modulus of the compositesincreases with an increase in mass fraction of polyvinyl alcohol.

Young's Modulus: It is defined as the ratio of stress and strain. It compares the relative stiffness of the composite. Figure 3 shows that the Young's modulus of the compositesincreases with an increase in mass fraction of polyvinyl alcohol.

Poisson Ratio: It is the ratio of lateral strain to longitudinal strain. Figure 4 shows that the Poisson ratio of the composite increases with an increase in mass fraction of polyvinyl alcohol.

Brittle Fracture Stress: Brittle Fracture is the sudden, rapid cracking of a material under stress where the material exhibited practically no evidence of ductility or plastic degradation before the fracture occurs. Figure 5 shows that the brittle fracture stress of the composite has no change with increase in mass fraction of acrylic acid

CONCLUSION

The possibility of the use of polyvinyl alcoholand polyethersulfone to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed concerning mechanical properties. The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio, and brittle stress fracture. The results indicated that the value of brittle stress fracture has no change and other properties increased with an increase in mass fraction of polyvinyl alcohol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money, and time.

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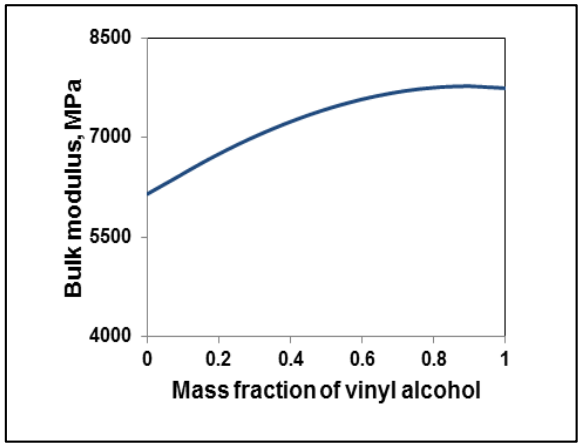

Figure1. Change in bulk modulus with the mass fraction of vinyl alcohol.

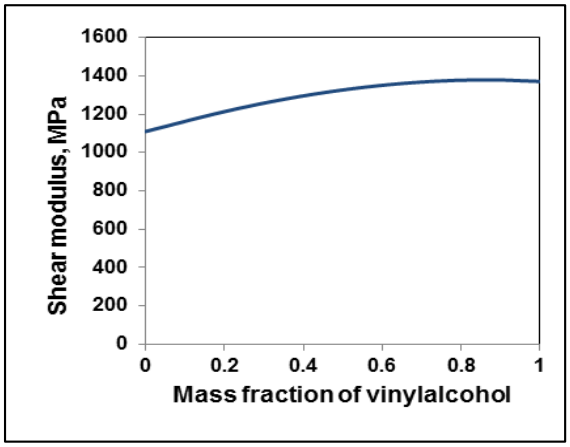

Figure2. Change in shear modulus with the mass fraction of vinyl alcohol.

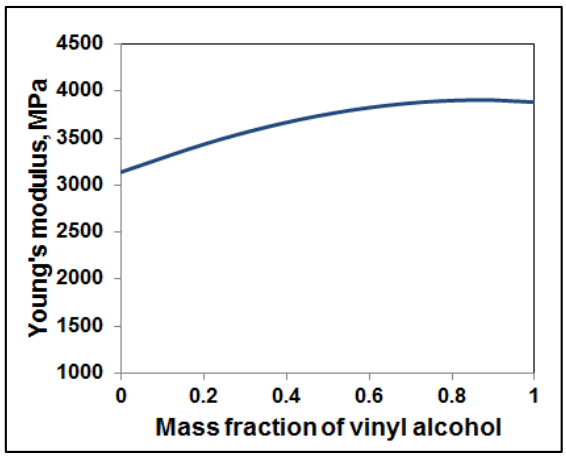

Figure3. Change in Young's modulus with the mass fraction of vinyl alcohol

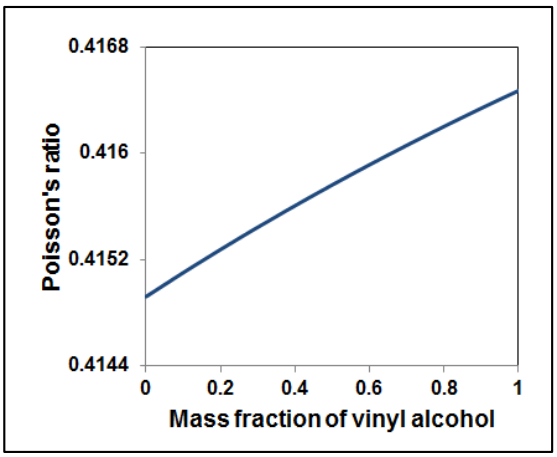

Figure 4. Change in Poisson modulus with the mass fraction of vinyl alcohol

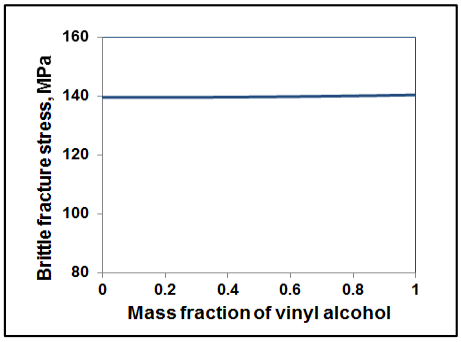

Figure 5. Change in brittle fracture with the mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyacrylic Acid and Poly Urea Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of polyacrylic acid and polyurea to provide desired mechanical properties of the blend was explored using Biovia Material Studio. The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio, and brittle stress fracture. The results indicated that the values of all the properties decreased with an increase in mass fraction of acrylic acid. This study will help determine pairs without performing laboratory experiments saving materials, money, and time.

Keywords: mechanical, in silico,polyacrylic acid, polyurea

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. The development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer. Nanomaterial modified polymers paved the way for multifunctional materials. Polymers coupled with carbon-based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fireproof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio

and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were developed for the construction of bridges, light rail transit, mining and tunneling, retaining walls, and other waterside buildings. All the above-mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time, and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs.

Acrylic polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects, etc. [8], bone repair [9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc. [10]. Polyacrylic acid is a polyelectrolyte soluble in aqueous media at neutral pH It is used for preparing hydrogels. It is not toxic and does not irritate [11]. This study is intended to identify the interaction of polyacrylic acid and polyurea to form blends. Polyurea is a type of elastomer that is derived from the reaction product of an isocyanate component and a synthetic resin blend component through step-growth polymerization. The isocyanate can be aromatic or aliphatic in nature. It can be monomer, polymer, or any variant reaction of isocyanates, quasi-prepolymer or a prepolymer. The prepolymer or quasi-prepolymer can be made of an amine-terminated polymer resin, or a hydroxyl-terminated polymer resin [12].

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and polyacrylochloride were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of the weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acidand polyurea as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Bulk Modulus: Bulk modulus is the measure of the decrease in volume with an increase in pressure. Figure 1 shows that the bulk modulus of the composite decreases with an increase in mass fraction of acrylic acid

Shear Modulus: It is defined as the ratio of shear stress and shear strain. It shows the response of the composite to shear deformation. Figure 2 shows that the shear modulus of the composite decreases with an increase in mass fraction of acrylic acid.

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Poisson Ratio: It is the ratio of lateral strain to longitudinal strain. Figure 4 shows that the Poisson ratio of the composite decreases with an increase in mass fraction of acrylic acid.

Brittle Fracture Stress: Brittle Fracture is the sudden, rapid cracking of a material under stress where the material exhibited practically no evidence of ductility or plastic degradation before the fracture occurs. Figure 5 shows that the brittle fracture stress of the composite decreases with increase in mass fraction of acrylic acid

CONCLUSION

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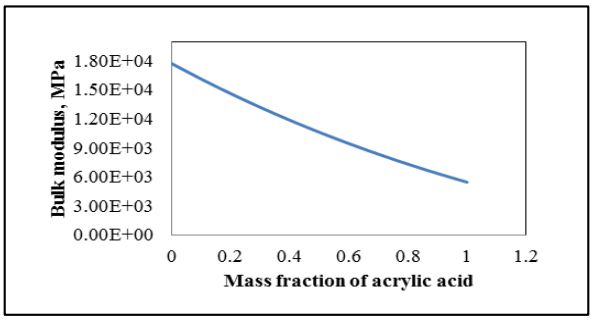

Figure 1. Change in bulk modulus with the mass fraction of acrylic acid

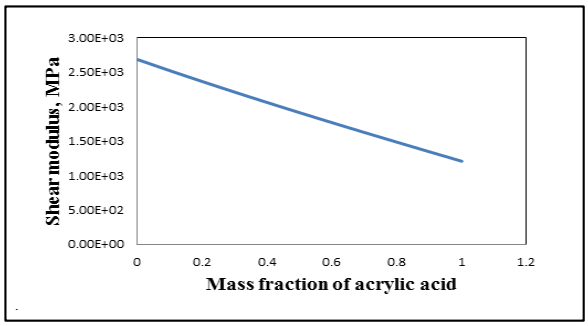

Figure 2. Change shear modulus with a mass fraction of acrylic acid

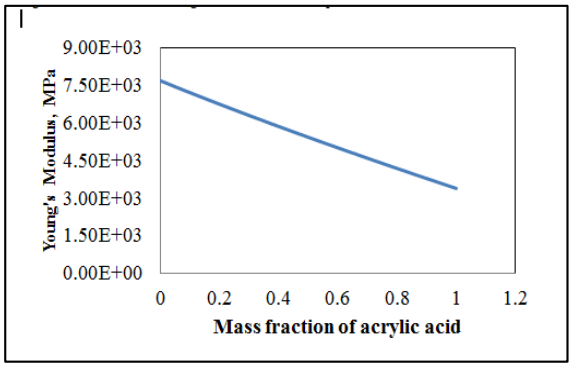

Figure 3. Change in Young's modulus with the mass fraction of acrylic acid

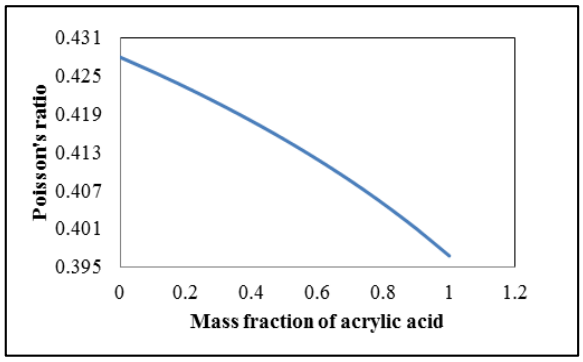

Figure 4. Change in Poisson modulus with the mass fraction of acrylic acid.

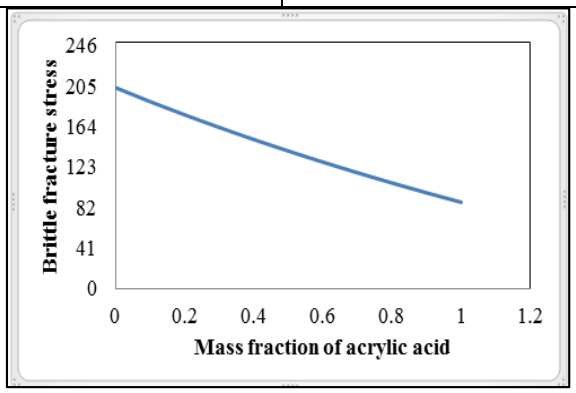

Figure 5. Change in brittle fracture with the mass fraction of acrylic acid.

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyvinyl Alcohol and Polyether Sulfone Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of the blend was analyzed concerning heat capacity, thermal conductivity, and dielectric constant. The results indicated that heat capacity and thermal conductivity decreased but dielectric constant increased with an increase in mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money, and time.

Keywords: thermal, dielectric,polyvinyl alcohol, in silico, polyethersulfone

INTRODUCTION

The blend may be a homogenous or heterogeneous mixture. Blends or composites are the physical combinations of more than one component where components do retain their identity in the mixture. A single material cannot provide multiple anticipated properties. It is desirable to combine different components thereby improving the properties of the material. The development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus blending is a process that provides an easy pathway to develop a new material by reducing the cost of development of products with preferred properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer. Polymers coupled with carbon-based (graphene, carbon nano-tube) nano-materials [1] have drawn significant attention in recent years. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fireproof materials [2]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4].

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RESULTS AND DISCUSSION

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To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Heat Capacity: It is the amount of heat required to raise the temperature of one unit weight of a substance by 1°C without change of phase. Figure 1 shows that the heat capacity (Cp) of the composite decreases with an increase in mass fraction of polyvinyl alcohol.

Thermal Conductivity: It indicates the correlation between heat flux per unit area and temperature gradient. It refers to the intrinsic ability of a material to transfer heat. Figure 2 shows that the thermal conductivity of the composite decreases with an increase in mass fraction of polyvinyl alcohol.

Dielectric Constant: It is defined as the ratio of the electric permeability of the material to the electric permeability of free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant. Figure 3 shows that the dielectric constant of the composite increases with an increase in the mass fraction of polyvinyl alcohol.

CONCLUSION

The possibility of the use of polyacrylic acid and polyurea to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed concerning heat capacity, thermal conductivity, and dielectric constant. The results indicated that heat capacity and thermal conductivity decreased but dielectric constant increased with an increase in mass fraction of polyvinyl alcohol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money, and time

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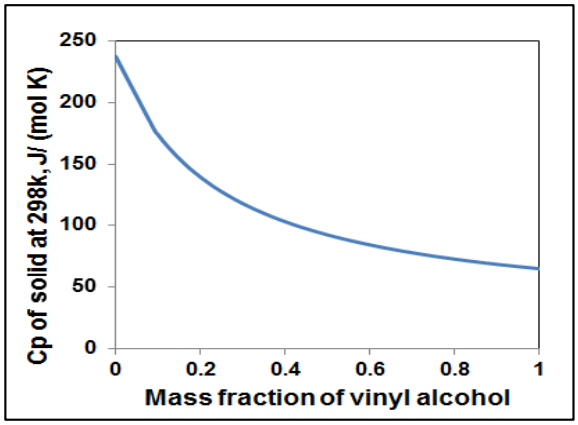

Figure 1. Change in heat capacity with the mass fraction of vinyl alcohol

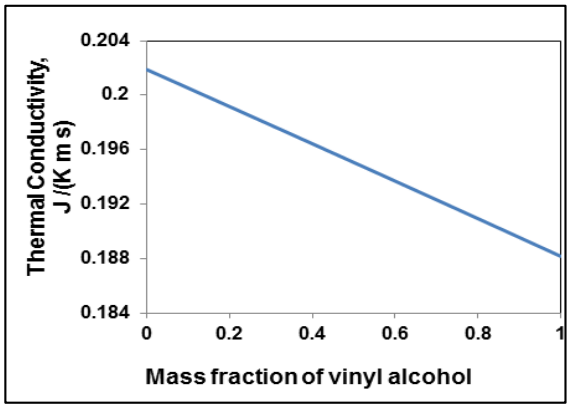

Figure 2. Change in thermal conductivity with the mass fraction of vinyl alcohol.

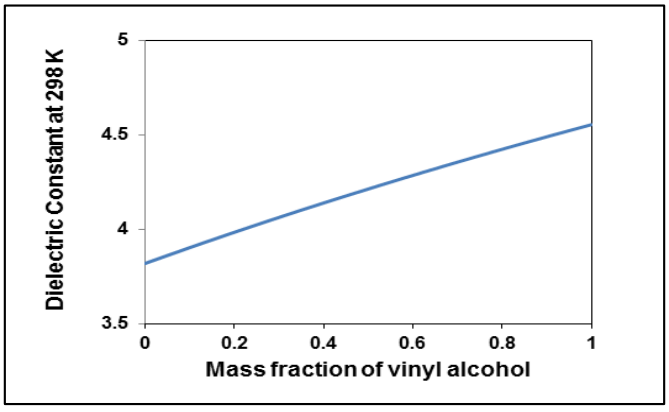

Figure 3. Change in Dielectric constant with the mass fraction of vinyl alcohol.

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyacrylic Acid and Polyurea Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of the blend was analyzed concerning heat capacity, thermal conductivity, and dielectric constant. The results indicated that heat capacity increased but thermal conductivity and dielectric constant decreased with an increase in mass fraction of polyacrylic acid. This study will help determine pairs without performing laboratory experiments saving materials, money, and time

Keywords: thermal, dielectric, polyacrylic acid, in silico, polyurea

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. The development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer. Nanomaterial modified polymers paved the way for multifunctional materials. Polymers coupled with carbon-based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fireproof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were developed for the construction of bridges, light rail transit, mining and tunneling, retaining walls, and other

waterside buildings. All the above-mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time, and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.

Acrylic polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects, etc. [8], bone repair [9], dispersing agent, super absorbent polymer, ion-exchange resin, etc. [10]. Polyacrylic acid is a polyelectrolyte soluble in aqueous media at neutral pH It is used for preparing hydrogels. It is not toxic and does not irritate [11]. This study is intended to identify the interaction of polyacrylic acid and polyurea to form blends. Polyurea is a type of elastomer that is derived from the reaction product of an isocyanate component and a synthetic resin blend component through step-growth polymerization. The isocyanate can be aromatic or aliphatic in nature. It can be monomer, polymer, or any variant reaction of isocyanates, quasi-prepolymer or a prepolymer. The prepolymer or quasi-prepolymer can be made of an amine-terminated polymer resin, or a hydroxyl-terminated polymer resin [12].

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and polyacrylochloride were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of the weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acidand polyurea as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Heat Capacity: It is the amount of heat required to raise the temperature of one unit weight of a substance by 1°C without change of phase. Figure 1 shows that the heat capacity (Cp) of the composite increases with an increase in mass fraction of acrylic acid.

Thermal Conductivity: It indicates the correlation between heat flux per unit area and temperature gradient. It refers to the intrinsic ability of a material to transfer heat. Figure 2 shows that the thermal conductivity of the composite decreases with an increase in mass fraction of acrylic acid.

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Dielectric Constant: It is defined as the ratio of the electric permeability of the material to the electric permeability of free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant. Figure 3 shows that the dielectric constant of the composite decreases with an increase in mass fraction of acrylic acid.

CONCLUSION

The possibility of the use of polyacrylic acid and polyureato form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed concerning heat capacity, thermal conductivity, and dielectric constant. The results indicated that heat capacity increased but thermal conductivity and dielectric constant decreased with an increase in mass fraction of polyacrylic acid. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money, and time.

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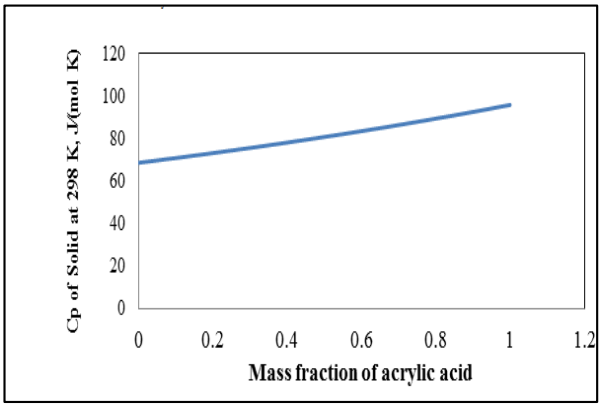

Figure 1. Change in heat capacity with the mass fraction of acrylic acid

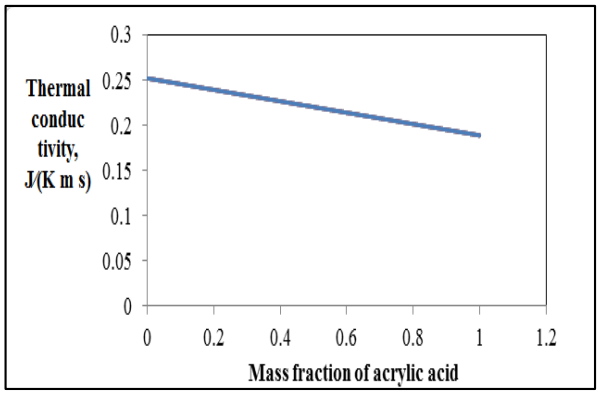

Figure 2. Change in thermal conductivity with the mass fraction of acrylic acid

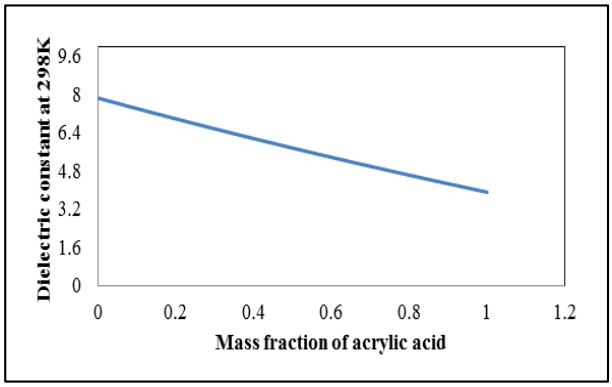

Figure 3. Change in Dielectric constant with the mass fraction of acrylic acid

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RESEARCH ARTICLE

In silico Analysis of Polyvinyl Alcohol and Poly Ethylene Terephthalate Compatibility in Blend

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ABSTRACT

A blend is created by the combination of two or more components. The compatibility of polyvinyl alcohol andpoly ethylene Terephthalate were study to form a miscible blend using Biovia Materials Studio. The compatibility of the two components was demonstrated based on free energy of combination, chi parameter, and mixing energy. The results indicated that the pair can become compatible only high temperature. Phasegraph indicated that a single phase can be obtained above 7500K which was the critical temperature. The coordination number was found to be 8.43 **+/-** 0.05. The highest number of configurations with respect to energy level was found to be -1.93Kal/Mol kcal/mol. This study will not only help to determine pairs without performing laboratory experiment but also less time consuming and low cost process.

Keywords: Blend; Insilico; Polyvinyl alcohol; Polyethylene terephthalate.

INTRODUCTION

Blends or composites are formed with combination of more than one component where components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisable to mix dissimilar components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of improvement of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material customized polymers paved the way to multi useful materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber

composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire evidence materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy lacking increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite material having high strength important for enhancing fuel efficiency in the field of transport [5]. There is application of composites in structural Engineering due to high strength to weight ratio and resistance to decay. Thus, glass fiber durable polymers, latex polymer cementations composites [6] were developed for building of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mention example relied on laboratory experiments.

Usually blends are prepared by test and fault method andthis method is a low cost and less time consuming method. Thus, researchers have focused on the use of in silicomove toward to develop new blends. Software (Materials Studio [7]) has been used to identify well-matched pairs. Among the a mixture of polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, simple film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is extensively used in covering industry to form strong polymeric films. It is because of their high mechanical power, environmental stability and easy processability [10]. On the other hand, PVA is poisonous, semicrystalline, hydrophilic, biocompatible and simply soluble in water [11].

The consumption of plastics in Western Europe is of 38 million tonnes per year, the majority of which are used in the production of plastic packaging, household and domestic products, electrical and electronic goods [12]. There is also significant consumption of plastics for the structure and construction industry and automotive industry. The two main types of plastics are thermoplastics, which soften when heated and harden again when cooled, and thermosets, which harden by curing and cannot be re-moulded. About 80 % of plastics used in Western Europe are thermoplastics [13].For many waste landfills is the largest route for disposal throughout the countries of Europe. For some countries, including Lithuania, more than 60 % of municipal solid waste is disposed of to landfill [14]. Plastics make up high proportion of waste that volume and range used increases dramatically. Although plastics make up between 5 wt.% and 15 wt.% of municipal solid waste it comprises 20 % – 30 % of the volume [13]. Most plastics are non-degradable and take a long time to decompose, possibly up to hundreds of years – although no-one knows for certain as plastics have not existed for long enough, when they are land filled. It is estimated that only about 50 % of the plastics produced in Western Europe each year are available for collection and recycling [12 – 14]. According to the experts from Kaunas University of Technology in Lithuania plastics reach about 82 thousands tones of municipal solid waste in 2004. It comprised about 24 kg for one inhabitant [15]. Waste recycling in Lithuania increases constantly and during 2000–2006 it ranges between 20 – 35 thousand tonnes per year [16]. According to the Environmental Protection Agency (EPA) "recycling" is considered to be processing of waste to make new article. There are divided three distinct approaches to the recycling of post-consumer plastic materials : 1) it could be reused directly; 2) undergo physical reprocessing, for example, grinding, melting and reforming; 3) be subjected to chemical treatment, when components are isolated and reprocessed for use in manufacture. A new widespread nomenclature of recycling was adopted by EPA. Primary recycling involves the use of pre-consumer industrial scrap and salvage, while physical reprocessing refers as secondary recycling and chemical processing as tertiary recycle [16].

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilize apparatus learning technique and standard algorithms to predict the level of communication.

Methodology: Polyvinyl alcohol andpoly ethylene Terephthalate to be prepared using the build menu of Materials Studio. The structures of the components were optimized using the mechanismto be used in blends->calculation menu of Materials studio. Polyvinyl alcohol was used as the base and poly ethylene Terephthalate was used as

screen. After estimate the blends->analysis menu of Materials studio was use to create various data. The data were analyzed and the compatibility of the mechanism to form a blend was analyzed.

RESULTS AND DISCUSSION

The use of polyvinyl alcohol and poly ethylene Terephthalate as potential mechanism of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: The blend is said to be miscible if it is homogeneous. A negative value of free energy of combination indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggest that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where ΔG_m = Gibb's free energy of mixing

ΔH_m = Enthalpy of mixing

ΔS_m = Entropy of mixing

T = Absolute temperature

The significance of $T\Delta S_m$ is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m at all times depends on the value of the enthalpy of mixing ΔH_m. The mechanism can mix to form a miscible blend only if the entropic contribution to free energy exceed the enthalpy contribution, i.e.,

$$\Delta H_m < T\Delta S_m \quad (2)$$

Figure 1 shows that the free energy involved in mixing is negative at around 140 Kandbeyong 500 K and positive for other temperature regeions studied here. The free energy decreases with increase in temperature (upto 140 K) as evident from Eq. 1 and free energy increases with increase in temperature after 145 K. then increase in the temperature it decreases gradually. The domino effect indicated that the mixture will take away to a identical mixture for the heat short 146K and beyond 500K. the trend shows a exceptionally agreeable compatibility between polyvinyl alcohol and polyethylene terephthalate with depressing significance of amalgamation energy for the above mentioned temperature.

Chi Parameter: The Flory-Huggins parameter describe the surplus free energy of combination and helps to explicate segment manner for polymer which are chemically similar, a momentous inequality in interrelated energy density leads to a extreme rate and, hence , a bigger pouring prize open for segment separation. So a exalted esteem of for chemically dissimilar polymers be a sign of meager mixing. For chemically comparable polymers having insignificant interrelated energy disaparity quantity is predictable to be small. However, nearby is a attempt of demixing for adequately lengthy chains. Architectural and numerical differences between the apparatus preclude them in a mixture from occupying the unaffected configuration accomplished in the nothing short of phase. Polymer area philosophy container predict that a difference in procession strength for chemically analogous machinery may pointer to a peak unquestionable importance of (chi).

Figure -2 shows that the set great store by is high point for the depths fever go and sad for the extreme hotness choice (500K) indicating amalgamation of the mechanism at high point temperature. The ⋅ merit decreased with raise in temperature. in this manner at important fever near is a leeway to variety a miscible blend. This agrees with the free energy of combination for the blend.

Coordination Number: The coordination number a_{ij} is the add up to of molecules of type 'j' that tin be packed around a lone molecule of type 'i'. the coordination number was calculate for each of the promising molecular pairs difficult in molecular simulations. The "Blends" module of materials studio differed from the Flory-Huggins from and second-hand an off-lattice calculation. It is understood that molecules are not agreed on a normal pattern as

probable in the creative Flory-Huggins theory. The coordination figure is large simply at what time the mechanism of the double mixture declares alike volumes or rise areas. It is intricate to rub on the pairs style in crucial a coordination add up to for a dual system in which the workings are not similar in size. In this look at carefully the coordination number was institute to be 8.43 +/- 0.05.

Energy Distribution for Blend: The group of unlike orientations via the pairs fashion may be the indication to configuration of unreliable energy levels. Figure 3 shows the plot of frequency (PE) against energy levels. It shows that the dissemination is rather irregular and at hand is a long, low-energy end. The quantity of configuration with energy higher than the peak respect decrease significantly.The maximum frequency was experiential for the energy level of around -1.93Kal/Mol .

Mixing Energy:A insignificant meaning of mixing energy preserve favors the mix process. Thus, the heat at which the incorporation energy is low container be elected for assimilation consider figure 4 shows the incorporation energy for the system was little for the high temperature studied. The diagram indicated that increase in temperature the addition energy up to 140K. it is and shows that combination energy steadily boost with add to fever after 140K up to 460K. So, it is same a large deal possible to the element at area of high pressure with superior amalgamation energy value

CONCLUSION

The scope of spending of polyvinyl alcohol and polyethylene terephthalate to custom a identical bring together was explored via Biovia material studio. The compatibility was analyzed based on free energy of mixing, inner self parameter and assimilation energy. The coordination come to was originate to be 8.43 +/- 0.05. the maximum number of configurations with think a lot of to energy smooth was bring into being -1.93Kal/Mol. As a rule apparatus for a mixture are identified experimentally this insillico study will did power mechanism of a mix together without performing arts laboratory experiment economy materials, funds and time.

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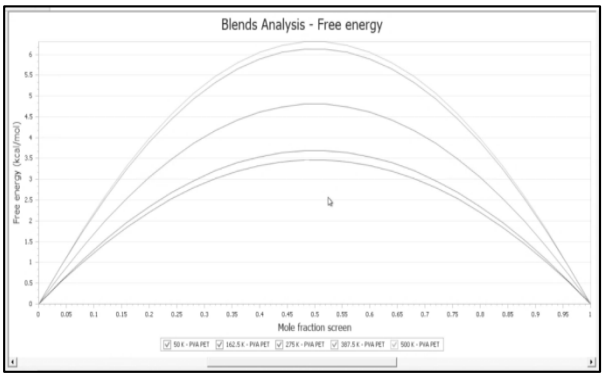

Figure 1. Free energy change with mole fraction of at polyethylene terephthalate different temperatures

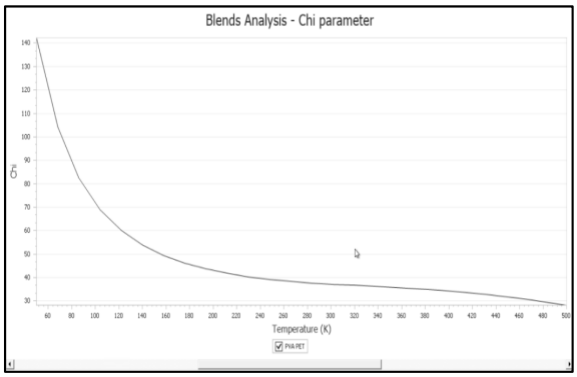

Figure 2. Change in χ (chi) value with temperature

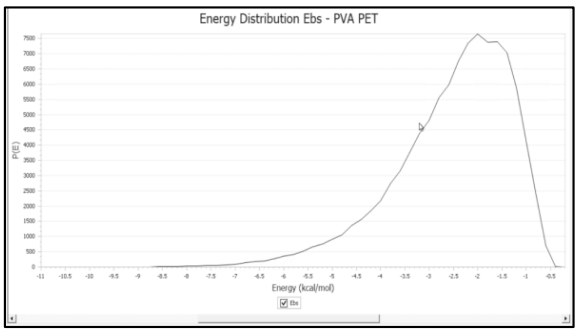

Figure-3 Energy distribution

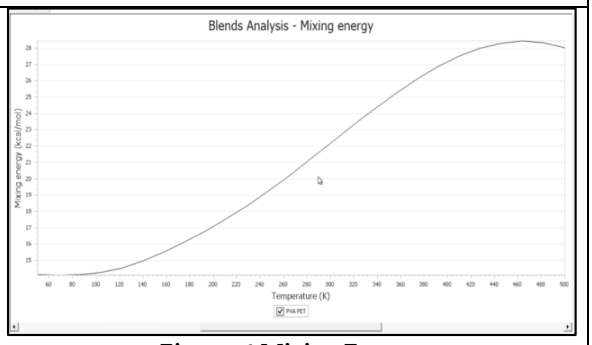

Figure -4 Mixing Energy

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RESEARCH ARTICLE

In silico Analysis of Polyacrylic Acid and Poly (Biphenyl Dimethyl Carbonate) Compatibility in a Blend

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ABSTRACT

This article intends to explore the compatibility of polyacrylic acid and poly(biphenyl dimethyl carbonate)to form a polymeric blend using Biovia Materials Studio.Polymeric blend is a physical combination of two or more polymers to develop hybrid polymer with enhanced properties. A blend may lead to Strong/weak molecular interaction to provide new properties which is desirable for various applications. The compatibility of the two components was studied based on the free energy of mixing, chi parameter, phase diagram, and mixing energy. The results indicated that the pair can become compatible only at high temperatures. Phase diagram indicated that a single phase can be obtained above 1350 K which was the critical temperature. The coordination number was found to be 7.84 +/- 0.05 The highest number of configurations for energy level was found to be -2.0 kcal/mol. The phase separation might lead to its use as porous material to be used as adsorbent. This study may help in determining the optimum composition/parameters required to prepare a homogeneous blend without performing laboratory experiments and therefore, saving materials, money, and time.

Keywords: Blend analysis, in silico, polyacrylic acid, poly-1, 2-α-D-glucose, biovia material studio, poly(biphenyl dimethyl carbonate)

INTRODUCTION

The blend may be a homogenous or heterogeneous mixture of more than one components with modified physical and chemical properties than the individual components. Blends or composites are the physical combination of more than one component where components do retain their identity in the mixture. A single material cannot provide multiple anticipated properties. It is desirable to combine different components thereby improving the properties of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus blending

is a process which provides an easy pathway develop a new material by reducing the cost of development of products with preferred properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer. A composite/ blend possess significantly different chemical and physical characteristics from those of its constituent components. In a composite the constituents remain physically separable and distinct from each other. Usually, a composite is a matrix in which strong and stiff reinforcement is distributed but made of a soft and weaker components [1-3]. The upgraded properties of composites are predominantly governed by their microstructure and interaction between matrix and reinforcing materials in the inter-phase region [4, 5]. Nano material modified polymers paved the way to multi functional materials.[6] Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [7] have drawn attention. Biodegradable polymers- natural fiber composites [8] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [9]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [10]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [11]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [12] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [13]) have been used to identify compatible pairs. Acrylic polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects etc. [14], bone repair [15], dispersing agent, superabsorbent polymer, ion-exchange resin, etc.[16].Polyacrylic acid is a polyelectrolyte soluble in aqueous media at neutral pH It is used for preparing hydrogels. It is not toxic and does not cause irritation [17].

Poly(biphenyl dimethyl carbonate) has an amorphous structure and is considered to be an engeeniering plastic. Its wide applications include impact resistance, strength, high temperature performance, toughness, load bearing capabilities, dimensional stability, flame retarding capabilities, and excellent optical clarity. Based on these properties they have commercialized as outdoor signs, eye glasses, compact disks, CD-ROM, aircraft windows, automotive windows and instrument panels, food trays and containers, automotive headlamp covers, housings of appliances, and medical devices [18, 19]. It has been found that biopolymer blends possess good thermal stability [20].This study is intended to identify the interaction of polyvinyl alcohol and poly biphenyl dimethyl carbonate to form blends. This study is intended to identify the interaction of polyacrylic acid and poly(biphenyl dimethyl carbonate) to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: Polyacrylic acid and poly (biphenyl dimethyl carbonate) were prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyacrylic acid was used as the base and poly (biphenyl dimethyl carbonate) was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acid and poly(biphenyl dimethyl carbonate) as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing:A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$\Delta G_m = \Delta H_m \quad T\Delta S_m$ (1)

where$\Delta G_m = Gibb's\ free\ energy\ of\ mixing$

$\Delta H_m - Enthalpy\ of\ mixing$

$\Delta S_m = Entropy\ of\ mixing$

$T = Absolute\ temperature$

The value of $T\Delta S_m$is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_malways depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$\Delta H_m < T\Delta S_m$ (2)

Figure 1 shows that the free energy involved in mixing is always positive for the temperatures studied. The free energy decreases with increase in temperature as evident from Eq. 1. The results indicated that the blend will not lead to a homogeneous mixture for the temperature range studied (50 to 500 K). The trend suggested that there might be a possibility of a miscible blend at very high temperature.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymershaving small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains.Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similarcomponentsmaylead to a high positive value of χ (chi).

Figure 2 shows that the χ value is high for the temperature range studied (50 to 500 K) indicating demixing. The χ value decreased with increase in temperature. Thus at high temperature there is a possibility to form a miscible blend. The result is in agreement with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size.In this study the coordination number was found to be7.84 +/- 0.05.

Phase Diagram: The compatibility of binary mixtures can be visualized by phase diagrams. Figure 3 shows the phase diagram for the two components of the blend. There are three regions of different degree of miscibility:

a. The single-phase miscible region existed above the critical temperatureof around 1350 K. This value supported the fact that a single phase blend can be formed at a high temperature (higher than 1350 K).

b. Fragmented metastable regions existedbetween binodals and spinodals, and

c. The two-phase separated regions of immiscibility are bordered by the spinodals.
The binodals separated miscible (one-phase) and metastable region, while the spinodals separated the metastable and two-phase region.
When the system enters from single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallizationi.e; slow nucleation followed by growth of the phase separated domains. On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distributionfor Blend: The generation of different orientations using the pairsmethod may lead to configurations of varying energy levels. Figure 4 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreasedsignificantly. The maximum frequency was observed for the energy level of around -2.0kcal/mol.

Mixing Energy:A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 5 shows that the mixing energy for the system was high for the temperature range studied. The graph indicated that an increase in temperature further leads to higher mixing energy. This result supported the previous observations. The formation of non homogeneous blend with polyacrylic acid as base might help formation of blend with higher porosity such as hydrogel. This might have an application as adsorbent.

CONCLUSION

The possibility of use of polyacrylic acid and poly(biphenyl dimethyl carbonate) to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible at high temperature. Phase diagram indicated that a single phase can be obtained above 1350 K. The coordination number was found to be 7.84 +/- 0.05 The maximum number of configurations with respect to energy level was found to be -2.0 kcal/mol.The phase separation might make it a porous material to be used as an adsorbent. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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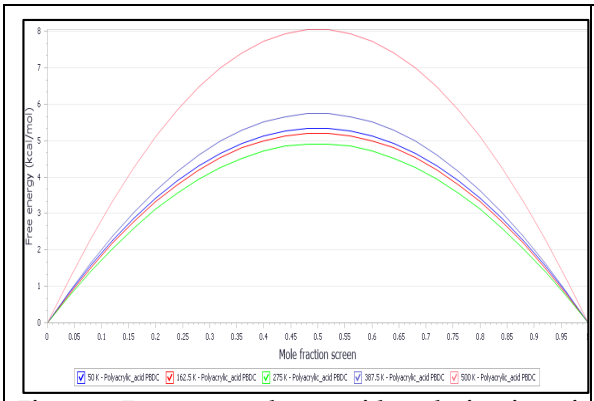

Figure 1. Free energy change with mole fraction of poly(biphenyl dimethyl carbonate) at different temperature

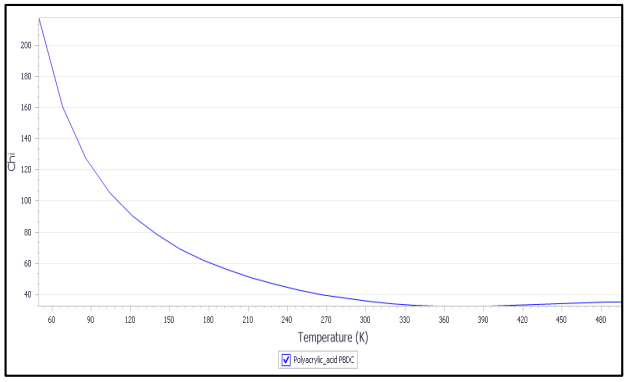

Figure 2. Change in χ (chi) value with temperature

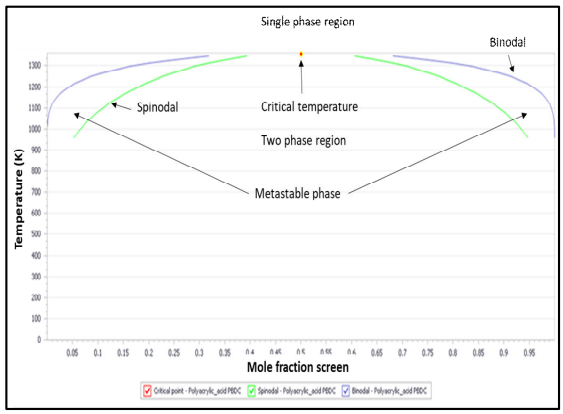

Figure 3. Phase diagram

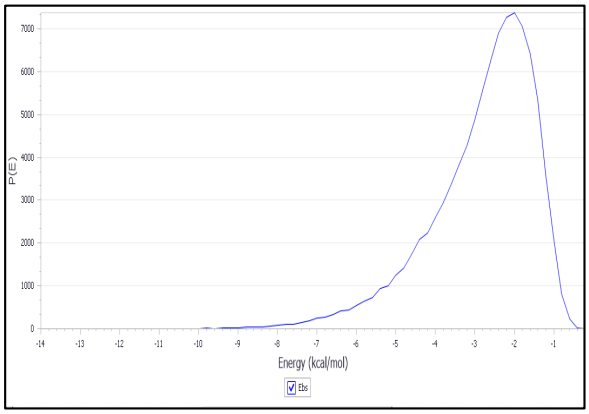

Figure 4. Energy distribution

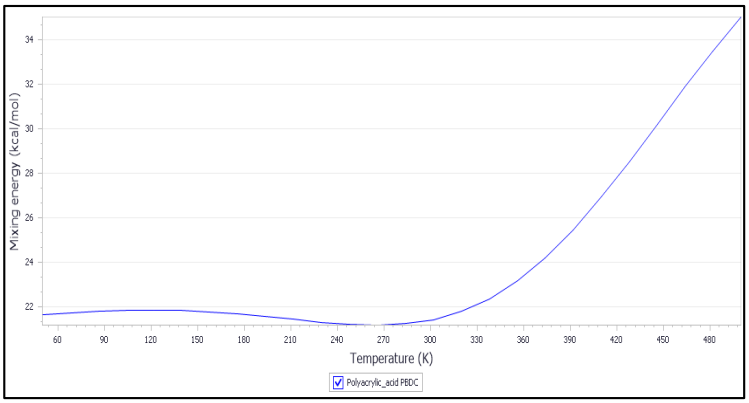

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyvinyl Alcohol Acid and Polybenzamide Compatibility in a Blend

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ABSTRACT

A blend is formed with the combination of two or more components. The compatibility of polyvinyl alcohol and polybenzamide were studied to form a miscible blend using Bio-via Materials Studio. The compatibility of the two components was demonstrated based on free energy of mixing, chi parameter, phase diagram and mixing energy. The results indicated that the pair can become compatible only at low temperature. Phase diagram indicated that a single phase can be obtained above 3900 K which was the critical temperature. The coordination number was found to be 6.62 +/- 0.04. The highest number of configurations with respect to energy level was found to be -2.30 kcal/mol. This study will not only help to determine pairs without performing laboratory experiments but also less time consuming and low cost process.

Keywords: Blend , in silico, polyvinyl alcohol, polybenzamide.

INTRODUCTION

Blends or composites are formed with combination of more than one component where components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisable to combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working

on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and fraction of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method andthis technique is a low cost and less time consuming method. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs. Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11].

The strategy used here for synthesis of poly(Benzamide)s relies on polymer end groups being more reactive than the monomer itself resulting in a kinetically controlled living chain-growth polymerization. Because of good control over the polydispersity and the molecular weight, a number of different polymer [12]. Specially synthesized rigid polybenzamide Nano whiskers of approximately 2000 nm length and 200 nm diameter were reported to increase tensile strength and Young's modulus without sacrificing high strain to-failure. [13]. This study is intended to identify the interaction of polyvinyl alcohol and polybenzamideto form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (DassaultSystemsof France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction

Methodology: Polyvinyl alcohol and polybenzamidewere prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyvinyl alcohol was used as the base and polybenzamidewas used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and polybenzamide as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where ΔG_m = *Gibb's free energy of mixing*

ΔH_m = *Enthalpy of mixing*

ΔS_m = *Entropy of mixing*

T = *Absolute temperature*

The value of $T\Delta S_m$ is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$\Delta H_m < T\Delta S_m$ (2)

Figure 1 shows that the free energy involved in mixing is negative at around 160 Kand beyong 500 K and positive for other temperature regeions studied here. The free energy decreases with increase in temperature (upto160 K) as evident from Eq. 1 and free energy increases with increase in temperature after 165 K upto 330 K.Furthet increase in the temperature it decreases gradually. The results indicated that the blend will not lead to a homogeneous mixture for the temperature range 161 K and beyond 500 K. The trend shows a very good compatibility between polyvinyl alcohol and poly polybenzamidewith negative value of mixing energy for the above mentioned temperatures, which may do not lead to form a perfect blend with significantly less effort.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similar components may lead to a high positive value of χ (chi). Figure 2 shows that the χ value is high for the low temperature range (500 K) .The χ value decreased in temperature. Thus at low temperature there is a possibility to form a miscible blend. This agrees with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It is assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size. In this study the coordination number was found to be 6.62 +/- 0.04.

Phase Diagram: The compatibility of binary mixtures can be visualized by phase diagrams. Figure 3 shows the phase diagram for the two components of the blend. There are three regions of different degree of miscibility:

a. The single-phase miscible region existed above the critical temperature of around 3900 K. This value supported the fact that a single phase blend can be formed at a high temperature (higher than 3900K).

b. Fragmented metastable regions existed between binodals and spinodals, and

c. The two-phase separated regions of immiscibility are bordered by the spinodals.

The binodals separated miscible (one-phase) and metastable region, while the spinodals separated the metastable and two-phase region.

When the system enters from single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e, slow nucleation followed by growth of the phase separated domains. On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 4 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -2.30 kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 6 shows that the mixing energy for the system was small for the temperature range studied. The graph indicated that an increase in temperature increased the mixing energy upto 220 K. It also shows that mixing energy gradually increases with decrease in temperature after 220 K upto 410 K and further increase in temperature the mixing energy increases. So, it is very much possible to mix the two components at high temperature with least mixing energy value. The formation ofhomogeneous blend with polyvinyl alcohol as base might help formation of blend with high mechanical strength. This might have an application as packaging material and adsorbent.

CONCLUSION

The possibility of use of polyvinyl alcohol and polybenzamide to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair can have very good compatibility at different ranges of temperature. The coordination number was found to be 6.62 +/- 0.04. The maximum number of configurations with respect to energy level was found to be -2.30 kcal/mol.Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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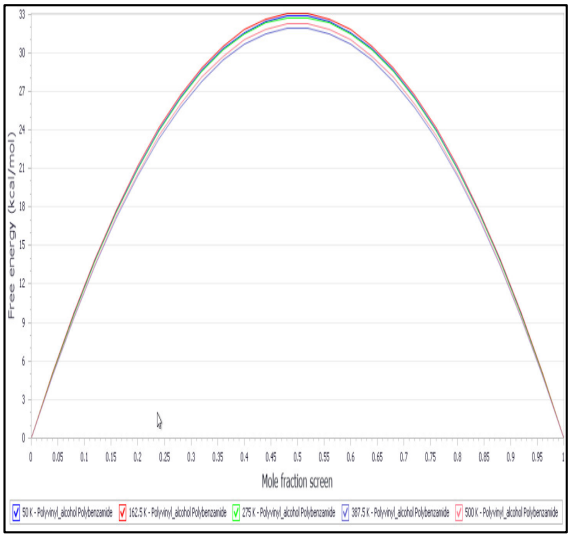

Figure 1. Free energy change with mole fraction of polybenzamide at different temperatures

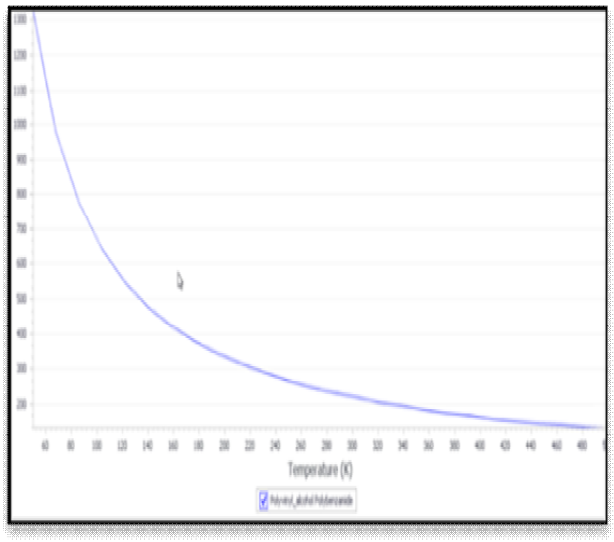

Figure 2. Change in χ (chi) value with temperature

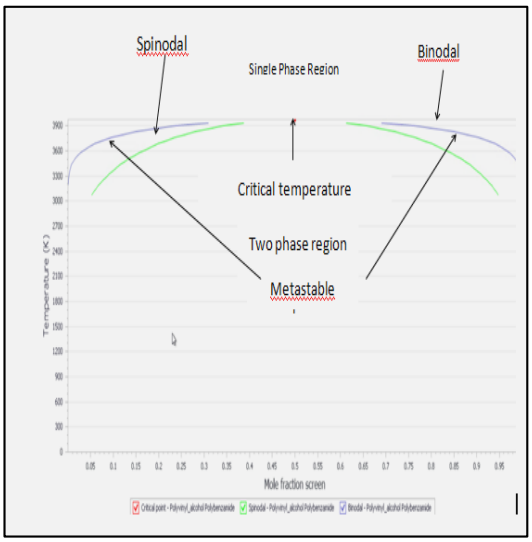

Figure 3. Phase diagram

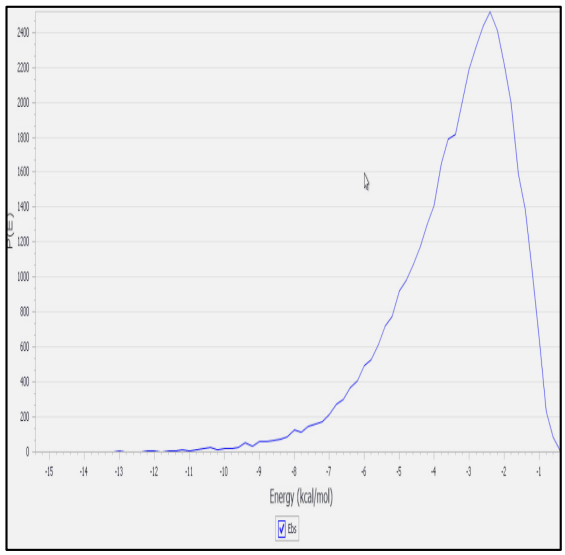

Figure 4. Energy distribution

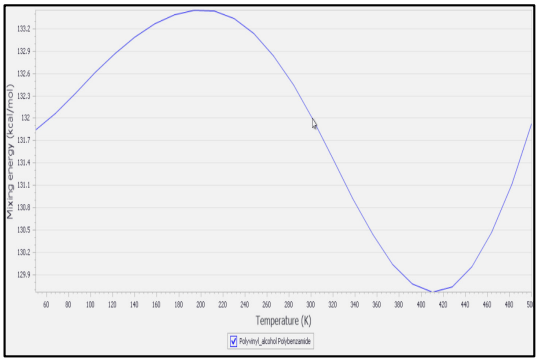

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyvinyl Alcohol Acid and Polybutylene Isopthalate Compatibility in a Blend

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ABSTRACT

A blend is formed with the combination of two or more components. The compatibility of polyvinyl alcohol and poly butylene isopthalate were studied to form a miscible blend using Biovia Materials Studio. The compatibility of the two components was demonstrated based on free energy of mixing, chi parameter, and mixing energy. The results indicated that the pair can become compatible only at high temperature. The coordination number was found to be 9.10 +/- 0.06. The highest number of configurations with respect to energy level was found to be -1.85kcal/mol. This study will not only help to determine pairs without performing laboratory experiments but also less time consuming and low cost process.

Keywords: Blend, in silico, polyvinyl alcohol, poly butylene isopthalate.

INTRODUCTION

Blends or composites are formed with combination of more than one component where components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisable to combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi-functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance

flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method and this technique is a low cost and less time consuming method. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs. Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11]. poly(butylene isophthalate) (PBI) are of potential interest as low melting temperature thermoplastics with adhesive properties. These materials are frequently referred to as "hot melts".[12].polybutylene isopthalate is a bio-based homo polymer, this polyester belongs to the class of poly (alkylene phthalate).the commercially use of PBI is based open its crystallization capability [13]. This aticle explores the compatibility of mixing of polyvinyl alcohol acid and polybutylene isopthalate in the temperature range of 50 K to 500 K.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: Polyvinyl alcohol and poly butylene isopthalate were prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyvinyl alcohol was used as the base and poly butylene isopthalate was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly butylene isopthalate as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where $\Delta G_m = Gibb's free energy of mixing$

$\Delta H_m = Enthalpy of mixing$

$\Delta S_m = Entropy of mixing$

$T = Absolute temperature$

The value of $T\Delta S_m$ is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$$\Delta H_m < T\Delta S_m \quad (2)$$

Figure 1 shows that the free energy involved in mixing is always positive for the temperature regions studied here (50-500). The results indicated that the blend will not lead to a hetrogeneous mixture for the temperature range studied (50 to 500 K). The trend shows a very less compatibility between polyvinyl alcohol and poly butylene isopthalate with positive value of mixing energy, which may lead to form a immiscible blend.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicates poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similar components may lead to a high positive value of χ (chi).

Figure 2 shows that the χ value is positive or high for the temperature range studied (50 to 500 K) indicating demixing. The χ value decreased with increase in temperature.Thus at high temperature there is a possibility to form a miscible blend beyond 500K.This agrees with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It is assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size. In this study the coordination number was found to be 9.10 +/- 0.06.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 5 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -1.85kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 6 shows that the mixing energy for the system was small for the temperature range studied. The graph indicated that an increase in temperature increased the mixing energy. It also shows that mixing energy gradually increases with increase intemperature upto 390 K, and starts decreasing beyond it. So, it is less possible to mix the two components at any feasible temperature with least mixing energy value. The formation of non homogeneous blend with polyvinyl alcohol as base might help formation of blend with high mechanical strength and porosity. This might have an application as packaging material and adsorbent.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly butylene isopthalate to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair may have less compatibility at different ranges of temperature. The coordination number was found to be 9.10 +/- 0.06. The maximum number of configurations with respect to energy level was found to be -1.85kcal/mol. Usually components for a blend are identified experimentally. This in silico

study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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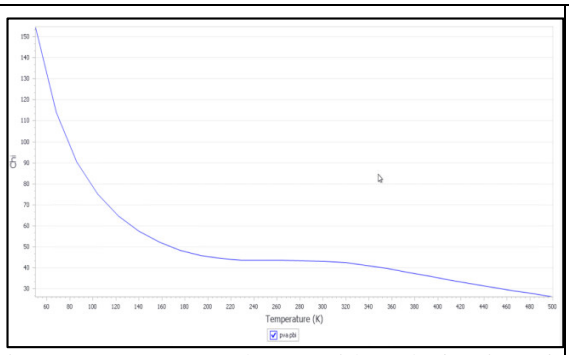

Figure 1. Free energy change with mole fraction of poly butylene isopthalateat different temperatures

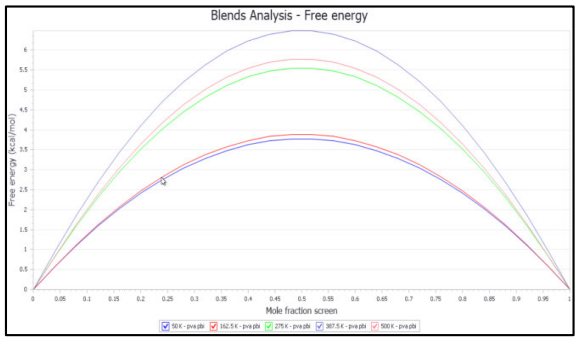

Figure 2. Change in χ (chi) value with temperature.

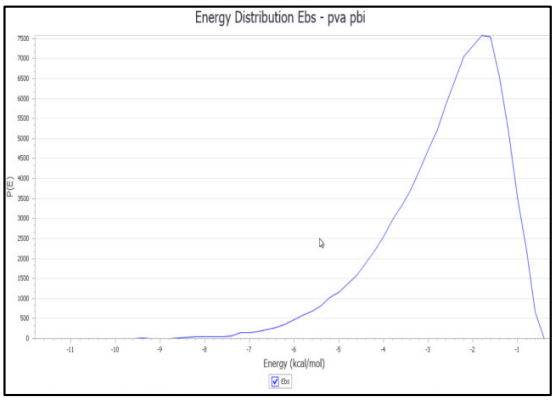

Figure 4. Energy distribution

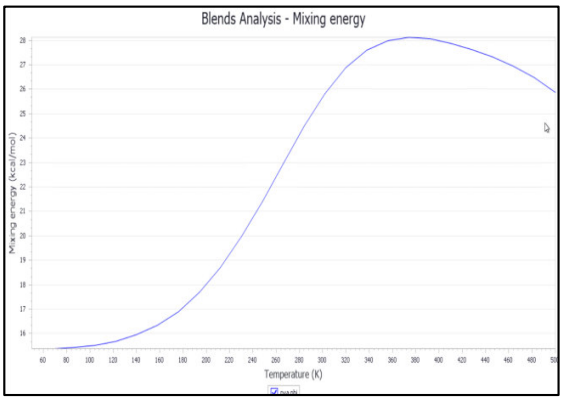

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyvinyl Alcohol Acid and Poly (Ether Sulfone) Compatibility in a Blend

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ABSTRACT

This manuscript is intended to explore the miscibility of polyvinyl alcohol and poly (ether sulfone) to form a polymeric blend using Biovia Materials Studio. The combination of two or more components is said to be a blend that may have the potential to display desirable properties. The compatibility of the two components was demonstrated based on the free energy of mixing, chi parameter, phase diagram, and mixing energy. The results indicated that the pair can become compatible only at high temperatures. The phase diagram indicated that a single phase can be obtained above 1280 K which was the critical temperature. The coordination number was found to be 8.70 +/- 0.05. The highest number of configurations with respect to energy level was found to be -2.0 kcal/mol. This study will not only help to determine pairs without performing laboratory experiments but also less time consuming and low-cost process

Keywords: Blend, in silico, polyvinyl alcohol, poly(ether sulfone), biovia material studio.

INTRODUCTION

The blend may be a homogenous or heterogeneous mixture. Blends or composites are the physical combinations of more than one component where components do retain their identity in the mixture.A single material cannot provide multiple anticipated properties. It is desirable to combine different components thereby improving the properties of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus blending is a process that provides an easy pathway to develop a new material by reducing the cost of development of products with preferred properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer. A composite/blend possesses significantly different chemical and physical characteristics from those of its constituent components. In a composite, the constituents remain physically separable and distinct from each other. Usually, a composite is a matrix in which strong and stiff reinforcement is distributed but made of soft

and weaker components [1-3].The upgraded properties of composites are predominantly governed by their microstructure and interaction between matrix and reinforcing materials in the inter-phase region [4, 5].Polymers coupled with carbon-based (graphene, carbon nano-tube) nano-materials [6] have drawn significant attention in recent years. Biodegradable polymers- natural fiber composites [7] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fireproof materials[8]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [9].

Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [10]. There are applications of composites in structural engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [11] were developed for the construction of bridges, light rail transit, mining and tunneling, retaining walls, and other waterside buildings. All the above-mentioned examples relied on laboratory experiments. Usually, blends are prepared by trial and error method and this technique is a low cost and less time-consuming method. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [12]) has been used to identify compatible pairs.

Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness, and whose properties can be controlled by do pant concentrations [13, 14]. The film-forming ability of PVA is widely used in the packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability, and easy process ability [15]. On the other hand, PVA is non-toxic, semi crystalline, hydrophilic, biocompatible, and easily soluble in water [16]. Polyether sulfone (PES) is one of the most important engineering polymeric materials. This polymer is extensively used in membrane separation devices, such as microfiltration and ultra filtration (UF) process in the fields of food, plasma separator, biomedicine, hemodialysis, and water purification, etc.[17-20]. In addition, it displays exceptional thermal, oxidative, and hydrolyticst ability as well as good mechanical and film-forming properties. It has been reported that blending PES with other polymers has addressed the surface physical and chemical properties with respect to improved membrane properties, modifications of the pore structure,etc. [21]. This study is intended to identify the interaction of polyvinyl alcohol and poly(ether sulfone) to form blends. A theoretical approach has been adopted to get the various parameters of blending without chemicals, experiments, and laboratory saving time, money, and energy.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: Polyvinyl alcohol and poly (ether sulfone) were prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyvinyl alcohol was used as the base and poly(ether sulfone)was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly (ether sulfone)as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$\Delta G_m = \Delta H_m \quad T\Delta S_m$ (1)

where ΔG_m = Gibb's free energy of mixing

ΔH_m = Enthalpy of mixing

ΔS_m = Entropy of mixing

T = Absolute temperature

The value of $T\Delta S_m$ is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$\Delta H_m < T\Delta S_m$ (2)

Figure 1 shows that the free energy involved in mixing is always positive for the temperature regions studied here (50 K to 500 K). The results indicated that the blend will lead to a heterogeneous mixture for the temperature range of 50 K to 500 K. The trend shows a very less compatibility between polyvinyl alcohol and poly(ether sulfone)with positive value of mixing energy for the above mentioned temperatures, which may lead to form a immiscible blend.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymers having small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains. Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similar components may lead to a high positive value of χ (chi).

Figure 2 shows that the χ value is high for the low temperature range and low for the high temperature range (500 K) indicating mixing of the components at high temperature. The χ value decreased with increase in temperature. Thus at high temperature there is a possibility to form a miscible blend (beyond 500 K). This agrees with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It is assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size. In this study the coordination number was found to be 8.70 +/- 0.05.

Phase Diagram: The compatibility of binary mixtures can be visualized by phase diagrams. Figure 3 shows the phase diagram for the two components of the blend. There are three regions of different degree of miscibility:

a. The single-phase miscible region existed above the critical temperature of around 1280 K. This value supported the fact that a single phase blend can be formed at a high temperature (higher than 1280K).

b. Fragmented metastable regions existed between binodals and spinodals, and

c. The two-phase separated regions of immiscibility are bordered by the spinodals.

The binodals separated miscible (one-phase) and metastable region, while the spinodals separated the metastable and two-phase region.

When the system enters from single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e, slow nucleation followed by growth of the phase separated domains. On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 4 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -2.0kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 6 shows that the mixing energy for the system was small for the temperature range studied. The graph indicated that an increase in temperature increased the mixing energy throughout the temperature range.So, it is very much possible to mix the two components at high temperature with high mixing energy value.

The formation of homogeneous blend with polyvinyl alcohol as base might help formation of blend with high mechanical strength. This might have an application as packaging material and adsorbent.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly(ether sulfone) to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair can have very good compatibility above 460 K. The coordination number was found to be 8.70 +/- 0.05. The maximum number of configurations with respect to energy level was found to be -2.0 kcal/mol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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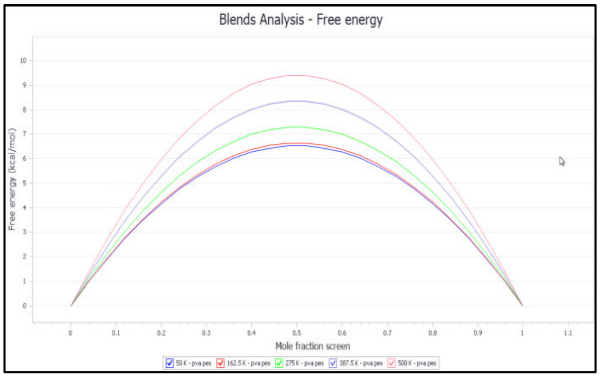

Figure 1. Free energy change with mole fraction of poly(ether sulfone) at different temperatures

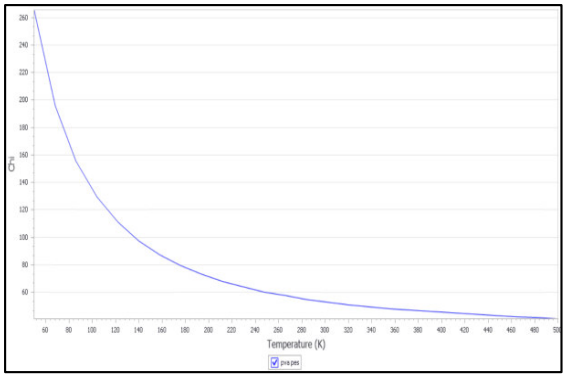

Figure 2. Change in χ (chi) value with temperature.

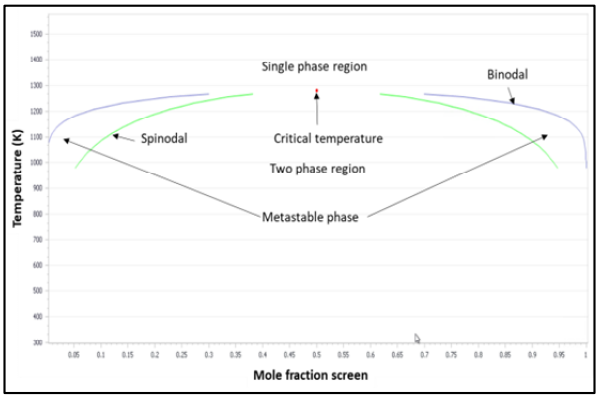

Figure 3. Phase diagram of the blend between polyvinyl alcohol and poly(ether sulfone).

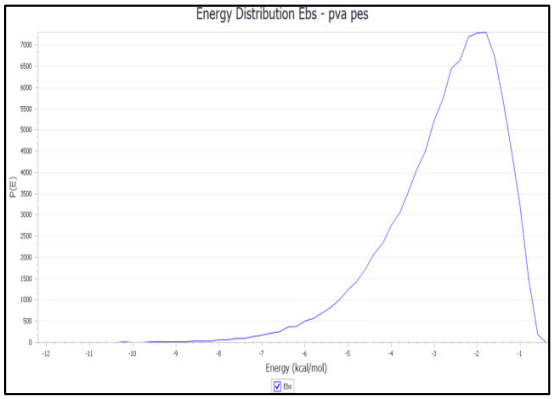

Figure 4. Energy distribution

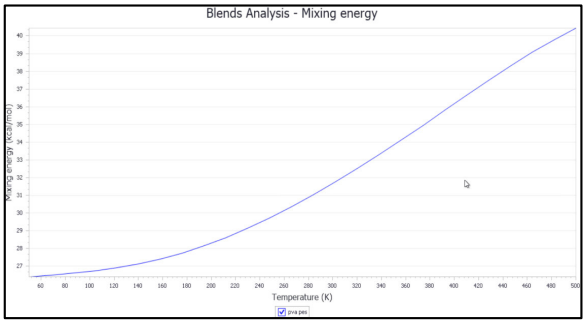

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyacrylic Acid and Poly Oxyetylene Comptibility in a Blend

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ABSTRACT

Usually blend is a combination of two or more mechanism and expected to have homogeneity. In this paper, we have tried to explore the compatibility of polyacrylic acid and poly oxyehylene to form a miscible blend using Biovia Materials Studio. The compatibility of the two components was studied based on free energy of mixing, chi parameter, and mixing energy. The results indicated that the pair can have very good compatibility at low to high temperature without any phase separation. The coordination number was found to be 5.23 +/- 0.03 . The highest number of configurations with respect to energy level was found to be -1.7Kal/Mol. This learning will help determine pairs without performing laboratory experiments saving resources, money and time.

Keywords: Blend; Insilico; Polyacrylic acid; Polyoxyethylene

INTRODUCTION

Blends or composite are resources containing more than one part. The components do retain their identity in the combination. As it is very difficult to find multiple properties in a single material, it is advisableto combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the preferred property. Thus a blend saves time to develop a new material thereby dipping the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn significant attention in recent years. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in

polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money.Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Acrylic acid have a board varity of application in dentistry as denture bases, artificial teeth , denture repair material, maxillofacial appliances for skeletal defects etc.[8] , bone repair [9] dispersing agent, superabsorbent polymer ion replaceresin, etc. [10] Polyacrylic acid is a polyelectrolyte soluble in aqueous media at impartial pH It is used for prepare hydrogels. It is not poisonous and does not reason irritation [11].

The area of high pressure molecular credence polymers deliberate were poly (oxythylene) homo polymers (polyox) with molecular with molecular credence ranging from 4,000,000 to 7,000,000 power characteristics optional fine flowability for these resources and predicted case fulfil importance uniformity irritation[12]. Experiments showed a precise extreme notch of bulge for these resources in equality gastric and shock absorber solution[13]. These polymers bottle sustain the discharge percentage of mutually water-soluble and indecipherable drugs from drug providing system. The soothing molecular burden polymers control a fewer marked sustained-release provoke compare to the eminent molecular authority polymer data (i.e individual with 7,000,000 molecular weight). Intensification in the freedom percentage of the drug. The solubility of the drugs openly influenced the make available rate. Discharge kinetics were evaluated and appeared to be influenced by the molecular import of the polymer, the solubility of medicine, and the ratio of the drug to the polymer in the capsule[14]. Biomodal issue kinetics was exhibit by a amount of furosemide formulation (i.e. F5and F8).

MATERIALS AND METHODS

Software Used: equipment studio module of Biovia software (Dassault Systemes of France) was used for study. The software utilizes appliance learning techniques and standard algorithms to predict the level of communication.

Methodology: Polyacrylic acid and poly oxyehylene were prepared using the build menu of resources Studio. The construction of the mechanism were optimized using the components were used in blends->estimate menu of Materials studio. Polyacrylic acid was used as the base and poly oxyethylene used as screen. After calculation the blends->analysis menu of Materials studio was used to make various data. The data were analyze and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this effort the use of polyacrylic acid and poly acrylic acid potential mechanism of a blend was analyzed by Biovia resources Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

Where ΔG_m = Gibbs free energy of mixing

ΔH_m = Enthalpyofmixing
ΔS_m = Entropyofmixing
T = absolute temperature

The value of $T\Delta S_m$is for all time positive in case of a blend since there is an increase in the entropy on addition. Therefore, the sign of ΔG_malways depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic involvement to free energy exceed the enthalpic contribution, i.e.,

$$\Delta H_m < T\Delta S_m \quad (2)$$

Figure 1 shows that the free energy involved in addition is always positive or greater than zero for the temperatures studied. The free energy decreases with increase in temperature as marked from Eq. 1. The results indicated that the blend is heterogeneous mixture for the temperature range studied (50 to 500 K). The trend show a very good compatibility among polyacrylic acid and poly oxyehylene with positive value of mixing energy.

Chi Parameter: The Flory–Huggins χ parameter describe the excess free energy of addition and helps to explain phase performance for polymer blends and block co polymers. For polymers which are not chemically similar, a important mismatch in cohesive energy density leads to a high χ value and, hence, a greater heavy force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymers having small cohesive energy variation χ value is probable to be small. However, there is a chance of demixing for adequately long chains.Architectural and geometric differences between the components check them in a combination from occupying the same configurations experience in the pure phase. Polymer field theory can predict that a difference in chain stiffness for chemically like components may lead to a high positive value of χ (chi).

Figure -2 shows that the superior inner self worth for the high temperature breadth international (50 to 500) indicating exact scanty mixing. The essence merit diminution with an intensification in heat up to 480K and the price practically remained unbroken with auxiliary increase in temperature. There is a lesser odd of identical incorporation with such amount of essence which agrees with the free energy of addition for the combination.

Coordination Number: The coordination number a_{ij} is the figure of molecules of type *j* that can be packed around a single molecule of type *i.* The coordination number was calculate for every of the possible molecular pairs involved in molecular simulation. The "Blends" module of equipment studio differed from the Flory-Huggins model and used an off-lattice estimate. It assumed that molecules are not set on a regular lattice as probable in the original Flory-Huggins theory. The coordination number is significant only when the mechanism of the binary blend have like volumes or surface areas. It is hard to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size.In this learning the coordination number was found to be5.23 +/- 0.03.

Phase Diagram: The compatibility of binary mixtures can be visualized by phase diagrams. Figure 3 shows the phase diagram for the two components of the blend. There are three regions of different degree of miscibility:
a. The single-phase miscible region existed above the critical temperature of around 800 K. This value supported the fact that a single phase blend can be formed at a high temperature (higher than 800 K).
b. Fragmented metastable regions existed between binodals and spinodals, and
c. The two-phase separated regions of immiscibility are bordered by the spinodals.
The binodals separated miscible (one-phase) and metastable region, while the spinodals separated the metastable and two-phase region.

When the system enters from single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e, slow nucleation followed by growth of the phase separated domains.

On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distribution for Blends: The making of something else orientation via the pairs technique may be in the lead to configuration of unreliable energy levels. Figure 4 shows the plot of frequency(PE) against energy levels. It shows the distribution is a small piece irregular and close to is a long, low energy extension. The come to of configuration with energy higher than the tip set great store by decreased significantly. The maximum frequency was experimental for the energy level of around -1.7Kal/Mol.

Mixing Energy: A little value of mixing energy can favor the addition process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 5 shows that the mixing energy for the system was small for the temperature range studied. The graph indicated that an increase in temperature increased the mixing energyfigure-5 shows that the combination energy for the system was minor for the passion collection studied. The chart indicated that an encourage in heat enlarged the combination energy. It in addition shows that assimilation energy will be no to around 210K, and the cost increasingly increase up to 9.6Kal/Mol at a temperature of 345K. However the amalgamation energy all over again reduces beyond the high temperature 345K. So, it is extremely a great deal likely to combine the two workings at any reasonable heat with slightest assimilation energy value. The formation of nonhomogeneous combine with polyacrylic acid as centre power good thing formation of balance with senior porosity such as hydrogel.

CONCLUSION

The possibility of use of polyacrylic acid and poly acrylic acid to form a homogeneous blend was explored using Biovia resources Studio. The compatibility was analyze based on free energy of addition, chi parameter and mixing energy. The results indicated that the pair can have less compatibility at different ranges of temperature. The coordination number was found to be 5.23 +/- 0.03 The maximum number of configurations with respect to energy level was found to be -1.7Kal/Mol Usually components for a blend are identified experimentally. This in silico study will help determine mechanism of a blend without performing laboratory experiments economy equipment, currency and time.

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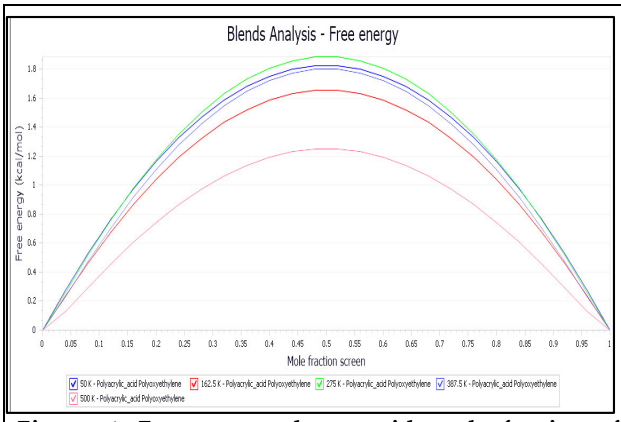

Figure -1: Free energy change with mole fraction of polyacrylic acid and polyoxythylene different temperature

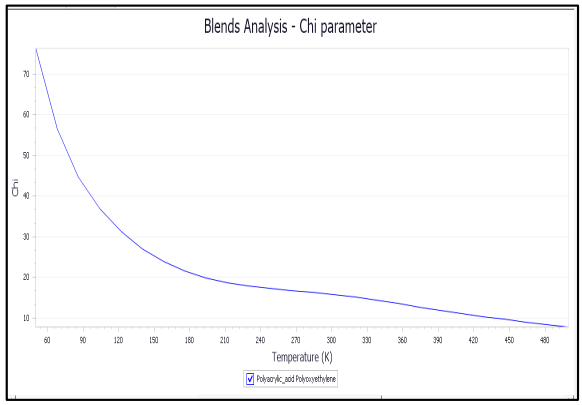

Figure -2 (change in (chi) value with temperature

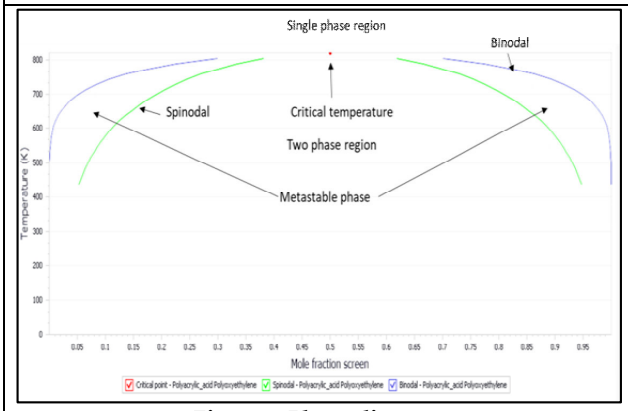

Figure-3:Phase diagram

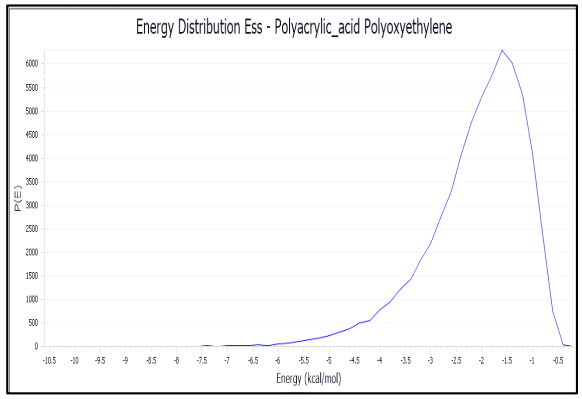

Figure-4: Energy distribution

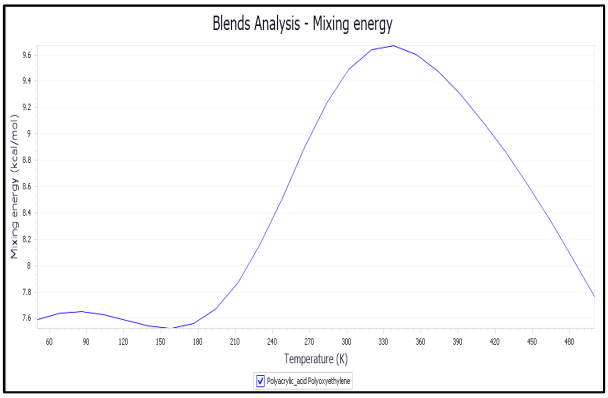

Figure-5: Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyacrylic Acid and Poly-1,2-α-D-Galactose Compatibility in a Blend

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ABSTRACT

Polyacrylic acid is a weak anionic polelectrolyte whose degree of ionization is pH dependant solution. In its non ionized form at low pHs, PAA may associate with various non ionic polymers. A blendis composition of two or more components and it is desirable to have homogeneityin a blend. In this article, we have tried to explore the compatibility of polyacrylic acid andPoly-1,2-*α*-D-galactoseto form a miscible blend using Biovia Materials Studio. The compatibility of the two components was studied based on free energy of mixing, chi parameter, and mixing energy. The results indicated that the pair can have very good compatibility at low to high temperature without any phase separation. The coordination number was found to be 6.46 +/- 0.03. The highest number of configurations with respect to energy level was found to be -2.1 kcal/mol. This study will help in determining the pairs without performing laboratory experiments saving materials, money and time.

Keywords: Blend, polyacrylic acid, Poly-1,2-*α*-D-galactose, in silico, Biopolymer

INTRODUCTION

Poly acrylic acid is a polyelectrolyte which is soluble in aqueous media at neutral pH due to the ionization of the pendent carboxyl side chains. Blends or composites are materials containing more than one component. The components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisableto combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nanomaterials have the ability to improve the properties of polymeric materials. Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancywithout increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money.Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7] have been used to identify compatible pairs.Acrylic polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects etc. [8], bone repair[9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc.[10].Polyacrylic acid is a polyelectrolyte soluble in aqueous media at neutral pH It is used for preparing hydrogels. It is not toxic and does not cause irritation [11].

Researchers have found applications of glycopolymers (synthetic polymers containing pendant carbohydrate groups) in the separation and removal of toxins and bacteria, tumor cell recognition and glucose-responsive insulin delivery [12].Glucose forms glycosidic bonds with itself, galactose to produce to nutritionally important disaccharides [13]. It has been found that biopolymer blends possess good thermal stability[14].This study is intended to identify the interaction of polyacrylic acid and Poly-1,2-α-D-galactoseto form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: Polyacrylic acid and Poly-1,2-α-D-galactosewere prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyacrylic acid was used as the base and Poly-1,2-α-D-galactosewas used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acid and Poly-1,2-α-D-galactoseas potential components of a blend was analyzed using Biovia Materials Studio.

Free energy of mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$\Delta G_m = \Delta H_m \quad T\Delta S_m$ (1)

where $\Delta G_m = Gibbs\ free\ energy\ of\ mixing$

$\Delta H_m = Enthalpy\ of\ mixing$

$\Delta S_m = Entropy\ of\ mixing$

T = Absolutetemperature

The value of $T\Delta S_m$is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_malways depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$\Delta H_m < T\Delta S_m$ (2)

Figure 1 shows that the free energy involved in mixing is always negative or less than zero for the temperatures studied. The free energy decreases with increase in temperature as evident from Eq. 1. The results indicated that the blend will absolutely lead to a homogeneous mixture for the temperature range studied (50 to 500 K). The trend shows a very good compatibility between polyacrylic acid and Poly-1,2-α-D-galactosewith negative value of mixing energy, which may lead to form a perfect blend with significantly less effort.

CHI Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymershaving small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains.Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similarcomponentsmaylead to a high positive value of χ (chi).

Figure 2 shows that the χ value is very small or negativefor the temperature range studied (50 to 500 K) indicating very good mixing. The χ value increased with an increase in temperature upto500 K. There is a very good possibility of homogeneous mixing with such small value of χ which agrees with the free energy of mixing for the blend.

Coordination number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size.In this study the coordination number was found to be6.46 +/- 0.03.

Energy distribution for blend: The generation of different orientations using the pairsmethod may lead to configurations of varying energy levels. Figure 3 shows the plot of frequency (P(E)) against energy levels. It shows that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreasedsignificantly. The maximum frequency was observed for the energy level of around -2.1kcal/mol.

Mixing energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 4 shows that the mixing energy for the system was small for the temperature range studied. The graph indicated that an increase in temperatureincreased the mixing energy. It shows that mixing energy gradually decreasingstarting from 50k up to 230K. However the mixing energy again increasesfrom 240K. So,it is very much possible to mix the two components at any feasible temperature with least mixing energy value. The formation of non homogeneous blend with polyacrylic acid as base might help formation of blend with higher porosity such as hydrogel. This might have an application as adsorbent.

CONCLUSION

The possibility of use of polyacrylic acid and Poly-1,2-α-D-galactoseto form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair can have very good compatibility at different ranges of temperature. The coordination number was found to be 6.46 +/- 0.03. The maximum number of configurations with respect to energy level was found to be-2.1 kcal/mol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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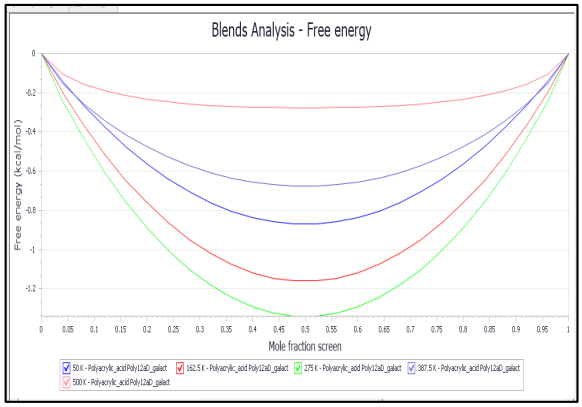

Figure 1. Free energy change with mole fraction of Poly-1,2-α-D-galactoseat different temperatures

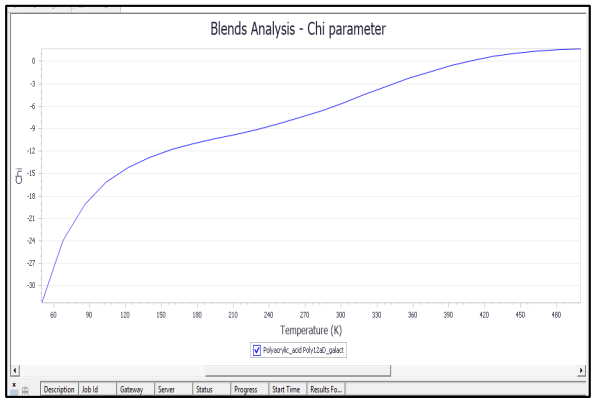

Figure 2. Change in χ (chi) value with temperature

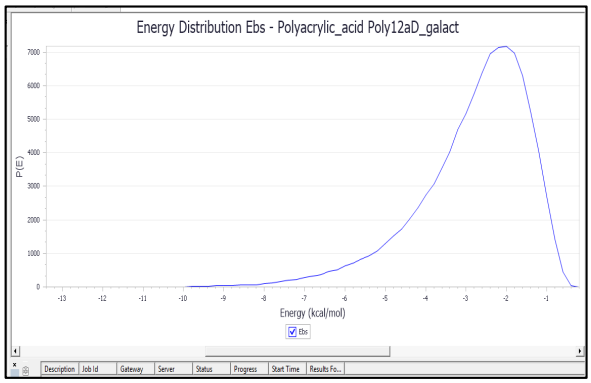

Figure 3. Energy distribution

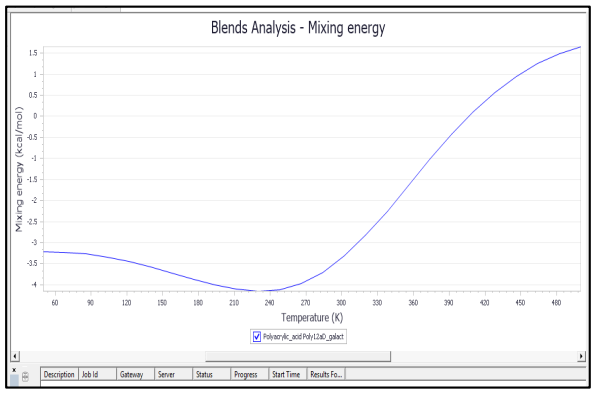

Figure 4. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyacrylic Acid and Poly-1,2-β-D-Galactose Compatibility in a Blend

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ABSTRACT

Polyacrylic acid is a weak anionic polelectrolyte whose degree of ionization is pH dependant solution. In its non ionized form at low pHs, PAA may associate with various nonionic polymers. A blendis always a composition of two or more components and it is desirable to have homogeneityin a blend. In this paper, we have tried to explore the compatibility ofpolyacrylic acid andpoly-1,2-β-D-galactoseto form a miscible blend using Biovia Materials Studio. The compatibility of the two components was studied based on free energy of mixing, chi parameter, and mixing energy. The results indicated that the pair can have very good compatibility at low to high temperature without any phase separation. The coordination number was found to be 7.41 +/- 0.04. The highest number of configurations with respect to energy level was found to be -2.0 kcal/mol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Blend, polyacrylic acid, poly-1,2-β-D-galactose, in silico, Biopolymer

INTRODUCTION

Biopolymers contain monomeric units that are covalently bonded to form larger structures. Biopolymers based on synthetic are used too manufacture many products of human use. Poly acrylic acid is a polyelectrolyte which is soluble in aqueous media at neutral pH due to the ionization of the pendent carboxyl side chains. Blends or composites are materials containing more than one component. The components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisableto combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancywithout increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

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Methodology: Polyacrylic acid and poly-1,2-β-D-galactosewere prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyacrylic acid was used as the base and poly-1,2-β-D-galactosewas used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acid and poly-1,2-β-D-galactoseas potential components of a blend was analyzed using Biovia Materials Studio.

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The value of $T\Delta S_m$is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_malways depends on the value of the enthalpy of mixingΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$$\Delta H_m < T\Delta S_m \quad (2)$$

Figure 1 shows that the free energy involved in mixing is always positive or more than zero for the temperatures studied. The free energy decreases with increase in temperature as evident from Eq. 1. The results indicated that the blend will absolutely lead to a homogeneous mixture for the temperature range studied (50 to 500 K). The trend shows a very good compatibility between polyacrylic acid and poly-1,2-β-D-galactose with positive value of mixing energy, which may lead to form a perfect blend with significantly less effort.

Chi parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymershaving small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains.Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similarcomponentsmaylead to a high positive value of χ (chi).

Figure. 2 shows that the χ value is very small in decreasing orderfor the temperature range studied (50 to 500 K) indicating very good mixing. The χ value gradually decreased in increase in tempreturestarting from 50K up to 500K. There is a very good possibility of homogeneous mixing with such small value of χ which agrees with the free energy of mixing for the blend.

Coordination number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size.In this study the coordination number was found to be7.41 +/- 0.04.

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Mixing energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 4 show that the mixing energy for the system was gradually increases with increase in temperature. The graph indicated that an increase in temperatureincreased the mixing energy. It also shows that mixing energy always positive from 50to 500 K, and the value gradually increases up to 26kcal/mol at a temperature of 500K. So, it is very much possible to mix the two components at any feasible temperature with least mixing energy value. The formation of nonhomogeneous blend with polyacrylic acid as base might help formation of blend with higher porosity such as hydrogel. This might have an application as adsorbent.

CONCLUSION

The possibility of use of polyacrylic acid and poly-1,2-β-D-galactoseto form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair can have very good compatibility at different ranges of temperature. The coordination number was found to be 7.41 +/- 0.04. The maximum number of configurations with respect to energy level was found to be -2.0 kcal/mol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time as well.

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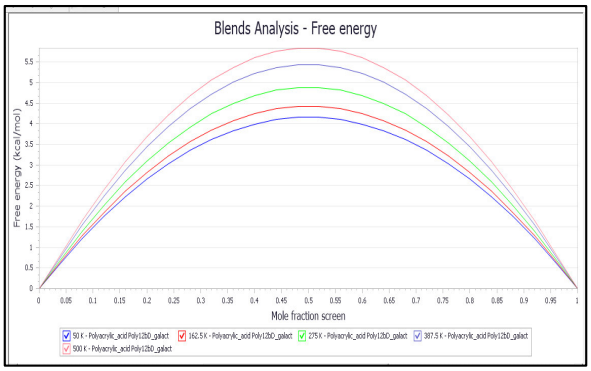

Figure 1. Free energy change with mole fraction of poly-1,2-β-D-galactoseat different temperatures

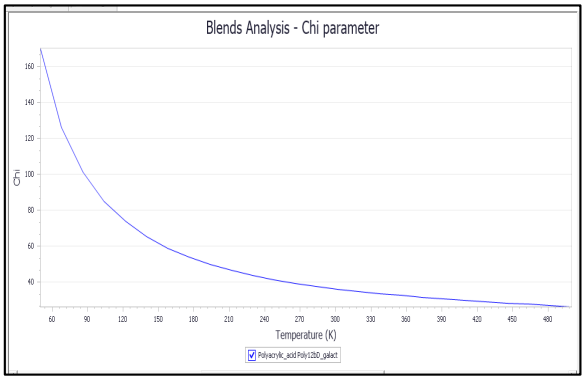

Figure 2. Change in χ (chi) value with temperature

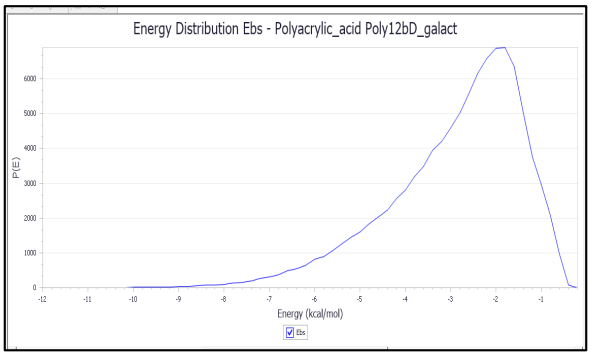

Figure 3. Energy distribution

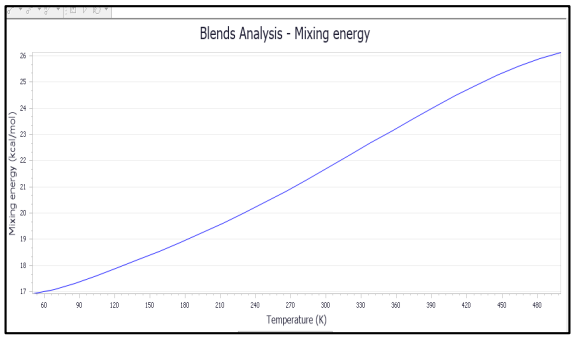

Figure 4. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Polyvinyl Alcohol and Poly (Biphenyl Dimethyl Carbonate) Compatibility in a Blend

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Received: 18 Mar 2020 Revised: 20 Apr 2020 Accepted: 22 May 2020

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ABSTRACT

Generally blend is a mixture of two or more components and expected to have homogeneity. In this paper, we have tried to explore the compatibility of polyvinyl alcohol and poly(biphenyl dimethyl carbonate)to form a miscible blend using Biovia Materials Studio. The compatibility of the two components was studied based on free energy of mixing, chi parameter, and mixing energy. The results indicated that the pair can have very good compatibility at low to high temperature without any phase separation. The coordination number was found to be 8.50 +/- 0.05. The highest number of configurations with respect to energy level was found to be -2.5 kcal/mol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Blend, in silico, polyvinyl alcohol, poly(biphenyl dimethyl carbonate), phase diagram

INTRODUCTION

Blends or composites are materials containing more than one component. The components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisableto combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi-functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn significant attention in recent years. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in

polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11].

Poly(biphenyl dimethyl carbonate) has an amorphous structure and is considered to be an engeeniering plastic. Itswide applicationsinclude impact resistance, strength, high temperatureperformance, toughness, load bearing capabilities, dimensional stability, flame retarding capabilities, and excellent optical clarity.Based on these properties they have commercialized asoutdoor signs, eye glasses, compact disks, CD-ROM, aircraft windows, automotive windows and instrument panels, food trays and containers, automotive headlamp covers, housings of appliances, and medical devices[12, 13]. It has been found that biopolymer blends possess good thermal stability [14].This study is intended to identify the interaction of polyvinyl alcohol and poly(biphenyl dimethyl cabonate)to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: Polyvinyl alcohol and polypoly(biphenyl dimethyl cabonate)were prepared using the build menu of Materials Studio. The structure of the components were optimized using the components were used in blends->calculation menu of Materials studio. Polyvinyl alcohol was used as the base and poly(biphenyl dimethyl carbonate)was used as screen. After calculation the blends->analysis menu of Materials studio was used to generate various data. The data were analyzed and the compatibility of the components to form a blend was analyzed.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly(biphenyl dimethyl carbonate)as potential components of a blend was analyzed using Biovia Materials Studio.

Free Energy of Mixing: A blend is said to be miscible if it is homogeneous. A negative value of free energy of mixing indicates that mixing is spontaneous and can lead to a homogeneous blend. Thermodynamic analysis suggests that

$$\Delta G_m = \Delta H_m - T\Delta S_m \quad (1)$$

where ΔG_m = Gibbs free energy of mixing

ΔH_m = Enthalpy of mixing

ΔS_m = Entropy of mixing

T = Absolute temperature

The value of $T\Delta S_m$ is always positive in case of a blend since there is an increase in the entropy on mixing. Therefore, the sign of ΔG_m always depends on the value of the enthalpy of mixing ΔH_m. The components can mix to form a miscible blend only if the entropic contribution to free energy exceeds the enthalpic contribution, i.e.,

$$\Delta H_m < T\Delta S_m \quad (2)$$

Figure 1 shows that the free energy involved in mixing is always positive and greater than zero for the temperatures studied. The free energy decreases with increase in temperature as evident from Eq. 1. The results indicated that the blend is a heterogeneous mixture for the temperature range studied (50 to 500 K). The trend shows a very good compatibility between polyvinyl alcohol and poly(biphenyl dimethyl carbonate) with positive value of mixing energy, which indicates that high energy is required to form a homogenous mixture.

Chi Parameter: The Flory–Huggins χ parameter describes the excess free energy of mixing and helps to explain phase behavior for polymer blends and block copolymers. For polymers which are not chemically similar, a significant mismatch in cohesive energy density leads to a high χ value and, hence, a greater driving force for phase separation. Thus a high value of χ for chemically dissimilar polymers indicate poor mixing. For chemically similar polymershaving small cohesive energy difference χ value is expected to be small. However, there is a chance of demixing for sufficiently long chains.Architectural and geometric differences between the components prevent them in a mixture from occupying the same configurations experienced in the pure phase. Polymer field theory can predict that a mismatch in chain stiffness for chemically similarcomponentsmaylead to a high positive value of χ (chi). The higher/positiveχ value for the temperature range studied (50 to 500 K) indicating very poor mixing (Figure 2). The χ value decreased with an increase in temperature upto260K and the value slightly increased and remained constant with further increase in temperature.There is a lesser possibility of homogeneous mixing with such value of χ which agrees with the free energy of mixing for the blend.

Coordination Number: The coordination number Z_{ij} is the number of molecules of type *j* that can be packed around a single molecule of type *i*. The coordination number was calculated for *each* of the possible molecular pairs involved in molecular simulations. The "Blends" module of Materials studio differed from the Flory-Huggins model and used an off-lattice calculation. It assumed that molecules are not arranged on a regular lattice as expected in the original Flory-Huggins theory. The coordination number is significant only when the components of the binary blend have similar volumes or surface areas. It is difficult to apply the pairs method in defining a coordination number for a binary system in which the components are not similar in size. In this study the coordination number was found to be8.50 +/- 0.05.

Phase Diagram: The compatibility of binary mixtures can be visualized by phase diagrams. Figure 3 shows the phase diagram for the two components of the blend. There are three regions of different degree of miscibility:
a. The single-phase miscible region existed above the critical temperature of around 1180 K. This value supported the fact that a single phase blend can be formed at a high temperature (higher than 1180 K).
b. Fragmented metastable regions existed between binodals and spinodals, and
c. The two-phase separated regions of immiscibility are bordered by the spinodals.
The binodals separated miscible (one-phase) and metastable region, while the spinodals separated the metastable and two-phase region.

When the system enters from single-phase region to the metastable region, the phase separation usually occurs by the mechanism of resembling crystallization i.e, slow nucleation followed by growth of the phase separated domains. On the other hand, when the system jumps from a single-phase into the spinodal region of immiscibility the phases separate spontaneously by a mechanism called spinodal decomposition.

Energy Distribution for Blend: The generation of different orientations using the pairs method may lead to configurations of varying energy levels. Figure 4 shows the plot of frequency (P(E)) against energy levels. It shows

that the distribution is somewhat asymmetrical and there is a long, low-energy tail. The number of configurations with energy higher than the peak value decreased significantly. The maximum frequency was observed for the energy level of around -2.5kcal/mol.

Mixing Energy: A small value of mixing energy can favor the mixing process. Thus, the temperature at which the mixing energy is low can be chosen for mixing. Figure 5 shows that the mixing energy for the system was small for the temperature range studied. The graph indicated that an increase in temperatureincreased the mixing energy. It also shows that mixing energy positive and decreases up to210 K, and the value gradually increases beyond temperature of220 K.This indicates the less possibility of mixing of these components in the temperature range of 50-500 K. The formation of non homogeneous blend with polyvinyl alcohol as base might help formation of blend with higher porosity such as hydro gel. This might have an application as adsorbent.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly(biphenyl dimethyl carbonate)to form a homogeneous blend was explored using Biovia Materials Studio. The compatibility was analyzed based on free energy of mixing, chi parameter and mixing energy. The results indicated that the pair can have less compatibility at different ranges of temperature. The coordination number was found to be 8.50 +/- 0.05. The maximum number of configurations with respect to energy level was found to be -2.5 kcal/mol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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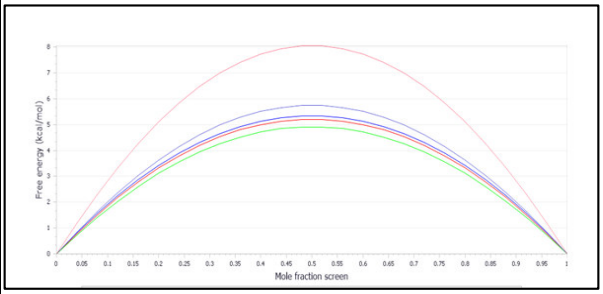

Figure 1. Free energy change with mole fraction of poly (biphenyl dimethyl carbonate)at different temperatures

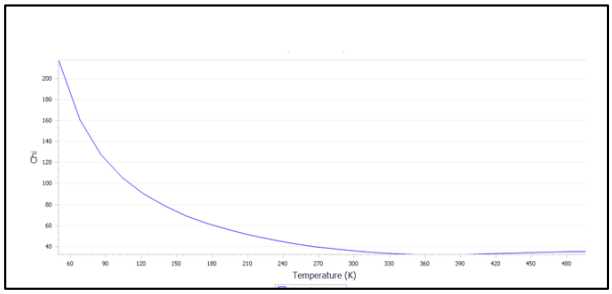

Figure 2. Change in χ (c hi) value with temperature

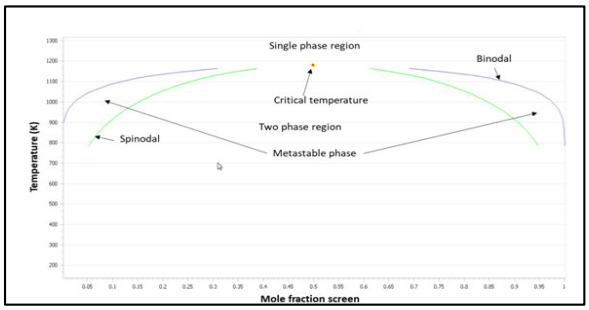

Figure 3. Phase diagram

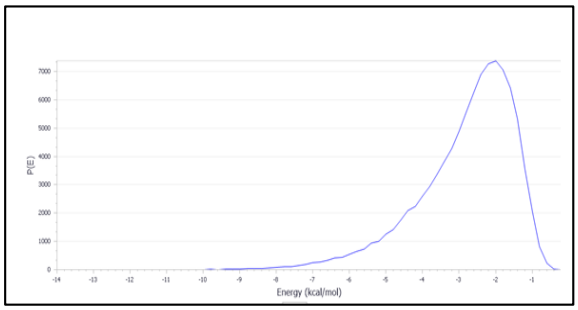

Figure 4. Energy distribution

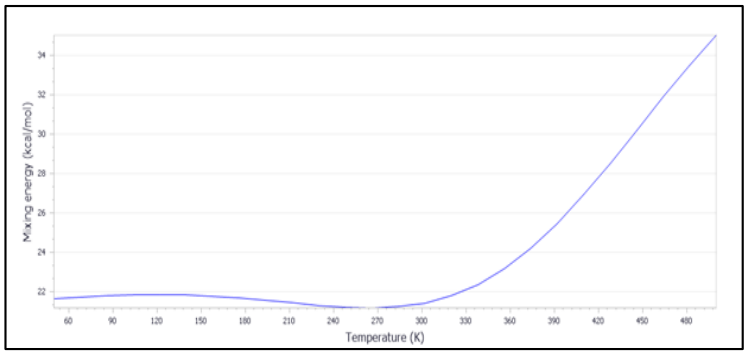

Figure 5. Mixing energy

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyvinyl Alcohol and Polybutyleneisopthalate Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of polyvinyl alcohol and and polybutylene isopthalate to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in polyvinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases decreased with increase in mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time

Keywords: Biovia, polyvinyl alcohol , polybutylene isopthalate

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of

lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11].poly(butylene isophthalate) (PBI) are of potential interest as low melting temperature thermoplastics with adhesive properties. These materials are frequently referred to as "hot melts"[12].Polybutylene isopthalate is a bio-based homo polymer, this polyester belongs to the class of poly (alkylene phthalate).the commercially use of PBI is based open its crystallization capability [13].

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and polybutylene isopthalate were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and Poly butylene isopthalate as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Density: Increase in density indicates decrease in porosity. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Permeability of gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium. Lower permeability indicates longer time lag for the gas to pass through the membrane. Figure 3 shows that the permeability of oxygen through the composite decreases with increase in mass fraction of vinyl alcohol.

Figure 4 shows that the permeability of nitrogen through the composite decreases with increase in mass fraction of vinyl alcohol. Figure 5 shows that the permeability of carbon dioxide through the composite decreases with increase in mass fraction of vinyl alcohol. Thus the results indicated that an increase in vinyl alcohol fraction reduces the permeability of different gases. The rate of permeability might be influence by the molecular weight of the gases.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly butylene isopthalateto form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in vinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeability for all the gases decreased with increase in mass fraction of vinyl alcohol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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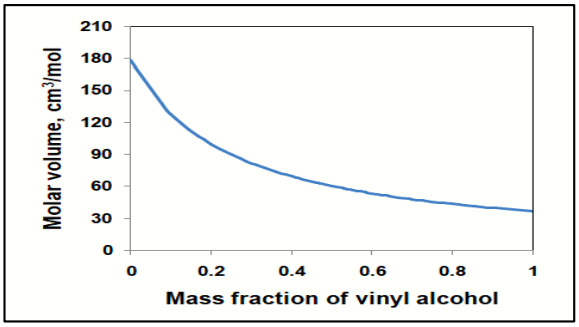

Figure 1. Change in molar volume with mass fraction of vinyl alcohol

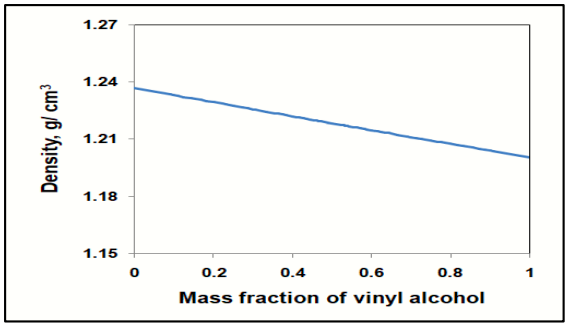

Figure 2. Change in density with mass fraction of vinyl alcohol

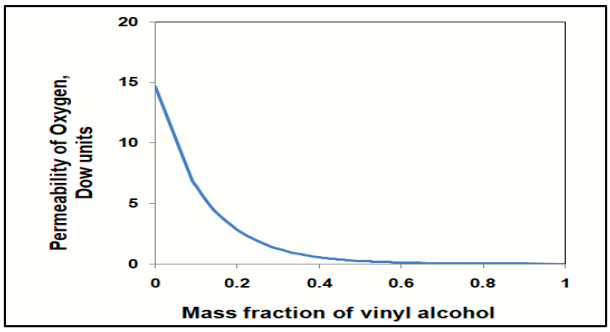

Figure 3. Change in permeability of oxygen with mass fraction of vinyl alcohol

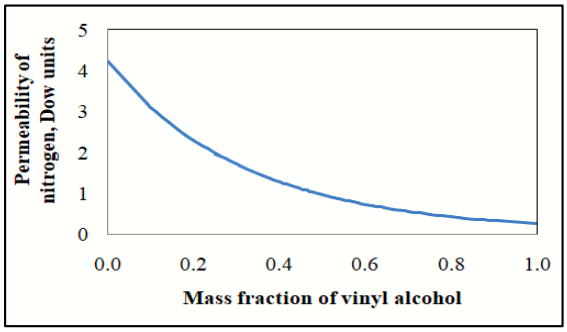

Figure 4. Change in permeability of nitrogen with mass fraction of vinyl alcohol

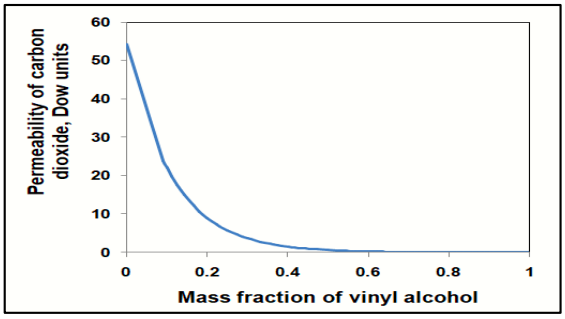

Figure 5. Change in permeability of carbon dioxide with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyvinyl Alcohol and Poly (Butylene Isophthalate) Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all those parameters increased with increase in mass fraction of vinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: *In silico*, thermal property, dielectric properties, polyvinyl alcohol, poly(butylene isophthalate), Synthia, Biovia

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi-functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio

and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs.

Acrylic polymers have a wide variety of applications in dentistry as denture bases, artificial teeth, denture repair materials, maxillofacial appliances for skeletal defects etc. [8], bone repair [9], dispersing agent, superabsorbent polymer, ion-exchange resin, etc.[10]. Polyvinyl alcohol is a polyelectrolyte soluble in aqueous media at neutral pH It is used for preparing hydrogels. It is not toxic and does not cause irritation [11]. poly(butylene isophthalate) (PBI) are of potential interest as low melting temperature thermoplastics with adhesive properties. These materials are frequently referred to as "hot melts".[12]. poly(butylene isophthalate) is a bio-based homo polymer, this polyester belongs to the class of poly (alkylene phthalate).the commercially use of PBI is based open its crystallization capability [13]. In this study the themal and dielectric properties of a blend between polyvinyl alcohol and poly(butylene isophthalate) are explored by using Biovia material studio.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction

Methodology: The structures of polyvinyl alcohol and poly (ethylene isophthalate) were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly (ethylene isophthalate) as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Heat capacity: It is the amount of heat required to raise the temperature of one unit weight of a substance by 1°C without change of phase. Figure 1 shows that the heat capacity (Cp) of the composite decreases with increase in mass fraction of vinyl alcohol.

Thermal conductivity: It indicates the correlation between heat flux per unit area and temperature gradient. It refers to the intrinsic ability of a material to transfer heat. Figure 2 shows that the thermal conductivity of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Dielectric constant: It is defined as the ratio of the electric permeability of the material to the electric permeability of free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant. Figure 3 shows that the dielectric constant of the composite increases with increase in mass fraction of vinyl alcohol.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly (ethylene isophthalate) to form a blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all the heat capacity and thermal conductivitydecreased with increase in mass fraction of vinyl alcohol whereas the dielectric constant decreased with it. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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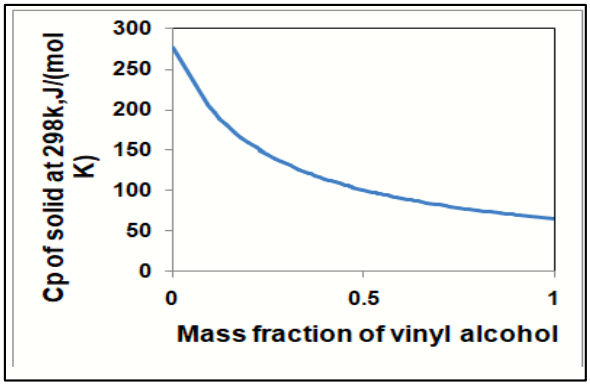

Figure 1. Change in heat capacity with mass fraction of vinyl alcohol

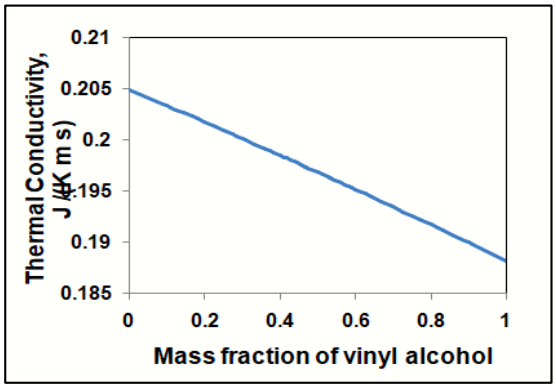

Figure 2. Change in thermal conductivity with mass fraction of vinyl alcohol

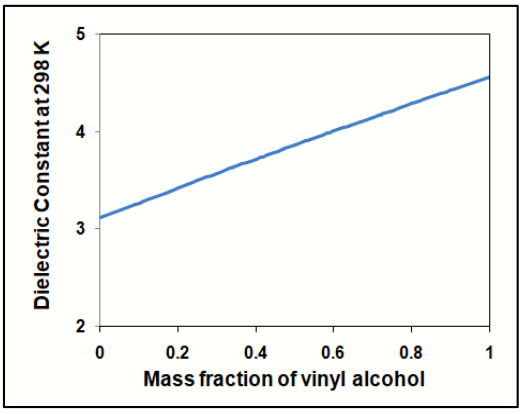

Figure 3. Change in dielectric constant with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyvinyl Alcohol and Polybutyleneisopthalate composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of polyvinyl alcohol and polybutyleneisopthalate to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of vinyl alcohol except Poisson ratio.This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Blend, Polyvinyl alcohol, Polybutyleneisopthalate

INTRODUCTION

Blends or composites are formed with combination of more than one component where components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisable to combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi-functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of

lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method and this technique is a low cost and less time consuming method. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs.

Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11].poly(butylene isophthalate) (PBI) are of potential interest as low melting temperature thermoplastics with adhesive properties. These materials are frequently referred to as "hot melts".[12]. poly(butylene isophthalate) is a bio-based homo polymer, this polyester belongs to the class of poly (alkylene phthalate).the commercially use of PBI is based open its crystallization capability [13].

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and polybutyleneisopthalate were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and polybutyleneisopthalate as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Bulk Modulus: Bulk modulus is the measure of the decrease in volume with an increase in pressure. Figure 1 shows that the bulk modulus of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Shear Modulus: It is defined as the ratio of shear stress and shear strain. It shows the response of the composite to shear deformation. Figure 2 shows that the shear modulus of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Young's Modulus: It is defined as the ratio of stress and strain. It compares the relative stiffness of the composite. Figure 3 shows that the Young's modulus of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Poisson Ratio: It is the ratio of lateral strain to longitudinal strain. Figure 4 shows that the Poisson ratio of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Brittle Fracture Stress: Brittle Fracture is the sudden, rapid cracking of a material under stress where the material exhibited practically no evidence of ductility or plastic degradation before the fracture occurs. Figure 5 shows that the brittle fracture stress of the composite increases linearly with increase in mass fraction of vinyl alcohol.

CONCLUSION

The possibility of use of polyvinyl alcohol and polybutyleneisopthalate to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to mechanical properties.The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of vinyl alcohol except Poisson ratio. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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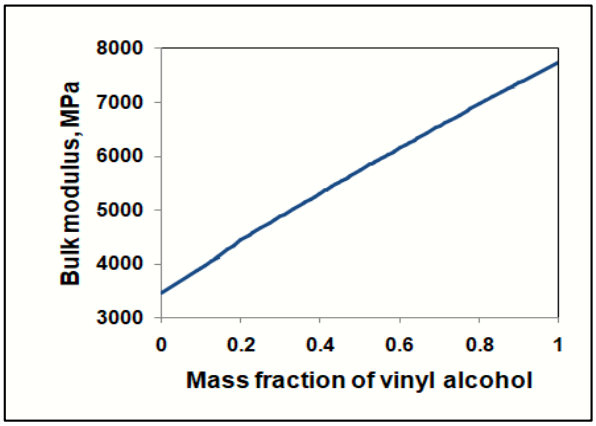

Figure 1. Change in bulk modulus with mass fraction of vinyl alcohol

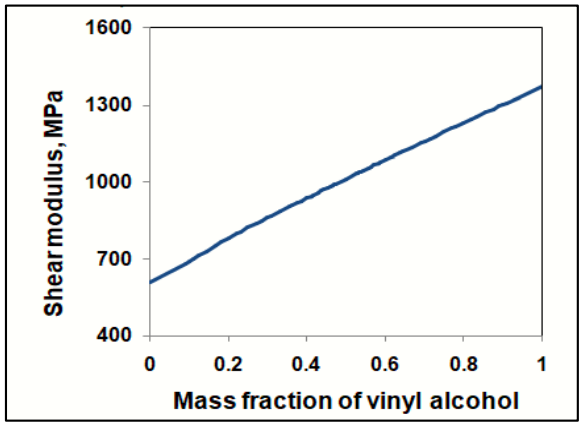

Figure 2. Change in shear modulus with mass fraction of vinyl alcohol

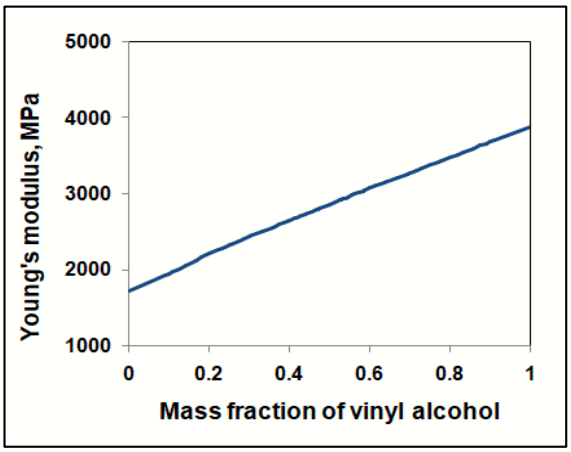

Figure 3. Change in Young's modulus with mass fraction of vinyl alcohol

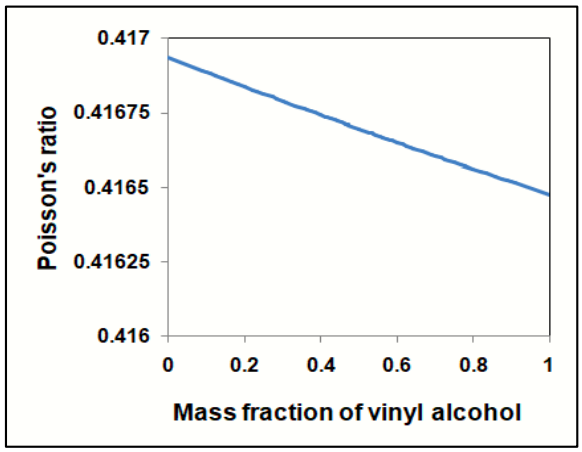

Figure 4. Change in Poisson modulus with mass fraction of vinyl alcohol

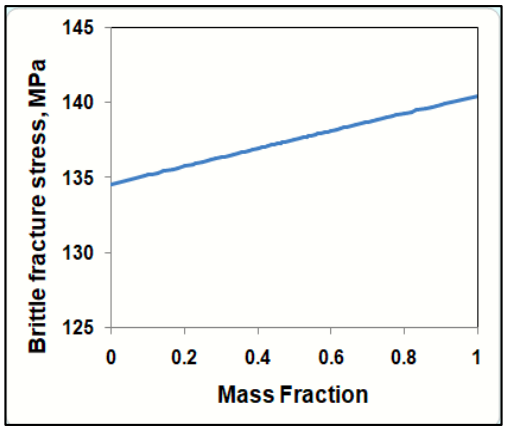

Figure 5. Change in brittle fracture stress with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyvinyl Alcohol and Poly (Biphenyl Dimethyl Carbonate) Composite

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ABSTRACT

Generally, blend is a mixture of two or more components and expected to have homogeneity. In this paper, we have tried to explore the compatibility of polyvinyl alcohol and poly (biphenyl dimethyl carbonate) to form a miscible blend using Biovia Materials Studio. The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of vinyl alcohol.This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: *In silico,* mechanical properties, polyvinyl alcohol, poly (biphenyl dimethyl carbonate), Biovia, Synthia

INTRODUCTION

Blends or composites are materials containing more than one component. The components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisable to combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

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Poly(biphenyl dimethyl carbonate) has an amorphous structure and is considered to be an engeeniering plastic. Its wide applications include impact resistance, strength, high temperature performance, toughness, load bearing capabilities, dimensional stability, flame retarding capabilities, and excellent optical clarity. Based on these properties they have commercialized as outdoor signs, eye glasses, compact disks, CD-ROM, aircraft windows, automotive windows and instrument panels, food trays and containers, automotive headlamp covers, housings of appliances, and medical devices [12, 13]. It has been found that biopolymer blends possess good thermal stability [14].This study is intended to identify the interaction of polyvinyl alcohol and poly(biphenyl dimethyl carbonate) to form blends. This study is intended to explore the mechanical properties of the blends developed by mixture of polyvinyl alcohol and poly(biphenyl dimethyl carbonate) using synthia tool.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction

Methodology: The structures of polyvinyl alcohol and poly(biphenyl dimethyl carbonate) were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly(biphenyl dimethyl carbonate) as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

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Brittle Fracture Stress: Brittle Fracture is the sudden, rapid cracking of a material under stress where the material exhibited practically no evidence of ductility or plastic degradation before the fracture occurs. Figure 5 shows that the brittle fracture stress of the composite increases linearly with increase in mass fraction of vinyl alcohol.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly(biphenyl dimethyl carbonate) to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to mechanical properties.The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of vinyl alcohol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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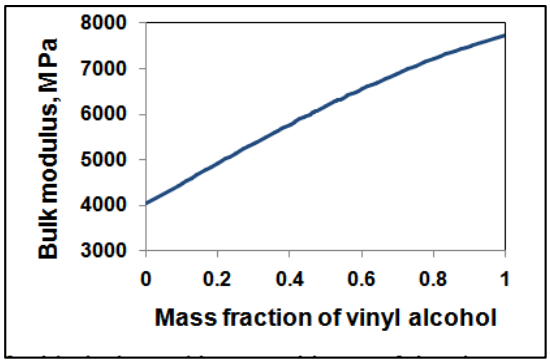

Figure 1. Change in bulk modulus with mass fraction of vinyl alcohol

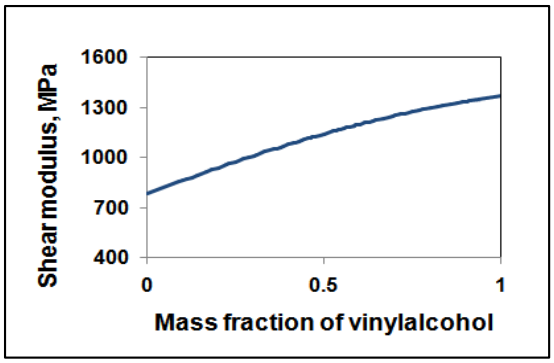

Figure 2. Change in shear modulus with mass fraction of vinyl alcohol

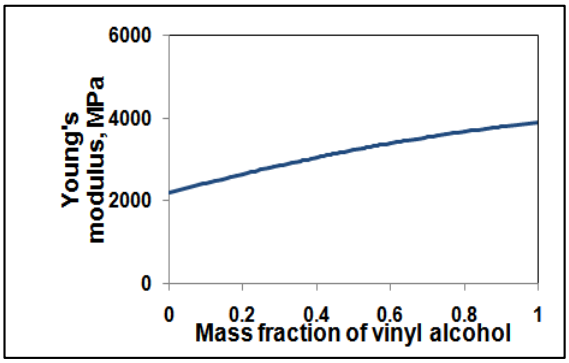

Figure 3. Change in Young's modulus with mass fraction of vinyl alcohol

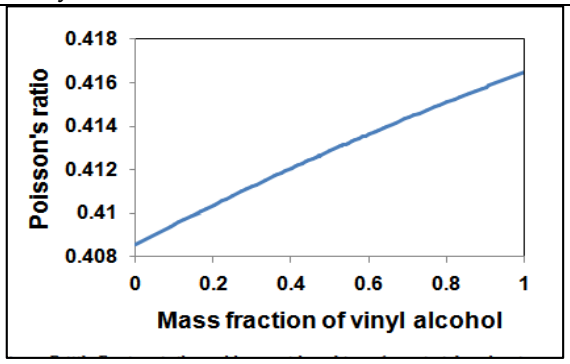

Figure 4. Change in Poisson modulus with mass fraction of vinyl alcohol

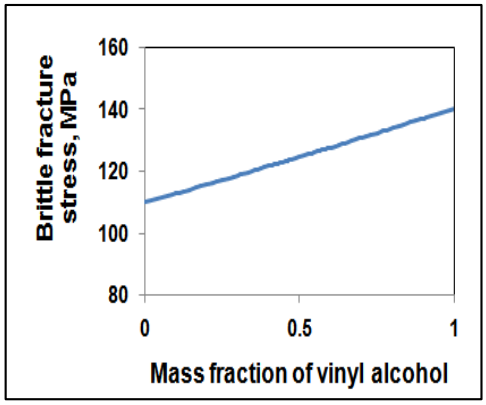

Figure 5. Change in brittle fracture stress with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyvinayl Alcohol and Polyethylene Terephthalate

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ABSTRACT

A blend is created bythe combination of two or more components. The compatibility of polyvinyl alcohol andpoly ethylene Terephthalate were study to form a miscible blend using Biovia Materials Studio. The mechanical properties of the composite to be studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The consequences indicated that the values of all the properties increased with increase in mass fraction of vinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, currency and time

Keywords: synthia, in silico, polyvinyl alcohol, polyethylene terephthalate.

INTRODUCTION

Blends or composites to be formed with combination of more than one component where components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisable to mix dissimilar components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilize the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of improvement of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material customized polymers paved the way to multi useful materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire evidence materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy lacking increasing the weight [4]. Researchers have emphasize on synthesis and production of lightweight composite material having high strength important for enhancing fuel efficiency in the

field of transport [5]. There are application of composites in structural Engineering due to high strength to weight ratio and resistance to decay. Thus, glass fiber durable polymers, latex polymer cementitious composites [6] were developed for building of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mention example relied on laboratory experiments. Usually blends are prepared by test and fault method andthis method is a low cost and less time consuming method. Thus, researchers have focused on the use of in silico move toward to develop new blends. Software (Materials Studio [7]) has been used to identify well-matched pairs. Among the a mixture of polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, simple film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is extensively used in covering industry to form strong polymeric films. It is because of their high mechanical power, environmental stability and easy processability [10]. On the other hand, PVA is poisonous, semicrystalline, hydrophilic, biocompatible and simply soluble in water [11].

The consumption of plastics in Western Europe is of 38 million tonnes per year, the majority of which are used in the production of plastic packaging, household and domestic products, electrical and electronic goods [12]. There is also significant consumption of plastics for the structure and construction industry and automotive industry. The two main types of plastics are thermoplastics, which soften when heated and harden again when cooled, and thermosets, which harden by curing and cannot be re-moulded. About 80 % of plastics used in Western Europe are thermoplastics [13].For many waste landfills is the largest route for disposal throughout the countries of Europe. For some countries, including Lithuania, more than 60 % of municipal solid waste is disposed of to landfill [14]. Plastics make up high proportion of waste that volume and range used increases dramatically. Although plastics make up between 5 wt.% and 15 wt.% of municipal solid waste it comprises 20 % – 30 % of the volume [13]. Most plastics are non-degradable and take a long time to decompose, possibly up to hundreds of years – although no-one knows for certain as plastics have not existed for long enough, when they are landfilled. It is estimated that only about 50 % of the plastics produced in Western Europe each year are available for collection and recycling [12 – 14].

According to the experts from Kaunas University of Technology in Lithuania plastics reach about 82 thousands tones of municipal solid waste in 2004. It comprised about 24 kg for one inhabitant [15]. Waste recycling in Lithuania increases constantly andduring 2000–2006 it ranges between 20 – 35 thousand tonnes per year [16]. According to the Environmental Protection Agency (EPA) "recycling" is considered to be processing of waste to make new article. There are divided three distinct approaches to the recycling of post-consumer plastic materials: 1) it could be reused directly; 2) undergo physical reprocessing, for example, grinding, melting and reforming; 3) be subjected to chemical treatment, when components are isolated and reprocessed for use in manufacture. A new widespread nomenclature of recycling was adopted by EPA. Primary recycling involves the use of pre-consumer industrial scrap and salvage, while physical reprocessing refers as secondary recycling and chemical processing as tertiary recycle [16].

MATERIALS AND METHODS

Software Used: equipment studio part of Biovia software (Dassault Systemes of France) was used for analysis. The software utilize machine study techniques and normal algorithms to predict the level of interaction.

Methodology: The structure of polyvinyl alcohol and poly ethylene Terephthalatewere fed to the synthia menu of equipment Studio. It was then run for different weight fractions of the mechanism. Different property of the composite was displayed in a tabular form. The values to be used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

The use of polyvinyl alcohol andpoly ethylene Terephthalate as potential mechanism of a composite was analyze using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-define correlation (advanced quantitative structure-property relationships) to estimate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. accordingly, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic relations that give rise to it. However, the main shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculate.To overcome this limitation, the technique implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from diagram theory are employed. The mechanical properties of the composite were premeditated based on size module, Bulk modules, Youngs modulus, Poission ratio and brittle stress fracture.

Bulk Modulus : The Bulk modulus of a substance is a measure of how resistance to compression that substance is. It is defined as the ratio of the infinitesimal pressure increase to the resulting relative to decrease of the volume. Figure 1 shows that the form modulus of the composite increase linearly with fuel in main part of poly vinayl alcohol.

Shear Modulus: The shear modulus is defined as the ratio of shear stress to shear strain. It is also known as modulus of rigidity. Figure 2 says that the modulus of rigidity of the composite increase with increase in ,ass fraction of polyvinayl alcohol

Young's Modulus: Young modulus, is a mechanical property that measures the stiffness of a solid material. Figure 3 shows that the Young's modulus of the composite increase with increase in mass fraction of poly vinayl alcohol

Poisson Ratio: Poisson's ratio is the ratio of transverse contraction strain to longitudinal extension strain in the direction of stretching force. Figure 4 shows that the Poisson ratio of the composite increase linearly with increase in mass fraction of poly acrylic acid.

Brittle Fracture Stress : A brittle fracture is the fracture of a metallic object or other material with appreciable prior plastic deformation. It is a break in a brittle piece of metal that failed because stress exceeded cohesion Figure 5 shows that the brittle fracture stress of the composite increase in increase in mass fraction of poly vinayl alcohol.

CONCLUSION

The preference of take advantages of polyacryalic acid and poly oxyethylene to a found a identical was explored by Biovia equipment studio. The organization of the balance was analyzed with think a lot of mechanical properties. The mechanical properties were considered based on substance modules, Young's modulus, Bulk modulus, Poisson ratio, shear modulus, brittle fracture. the result indicated that the values of all the properties increase and increase with increase in mass fraction of polyvinayl alcohol. This in silico revision will comfort govern mechanism of a mix together without the stage laboratory experiments economy materials, money and time.

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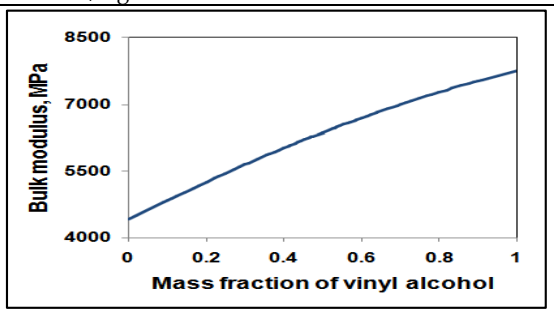

Figure 1. Change in bulk modulus with mass fraction of poly acrylic acid.

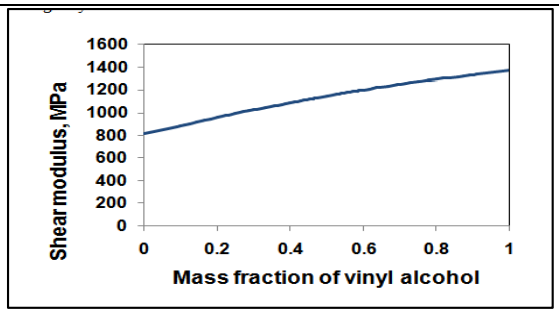

Figure 2. Change in shear modulus with mass fraction of polyvinayl alcohol

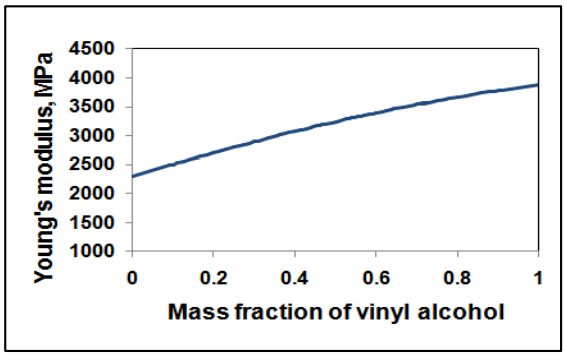

Figure 3. Change in Young's modulus with mass fraction of poly vinayl alcohol

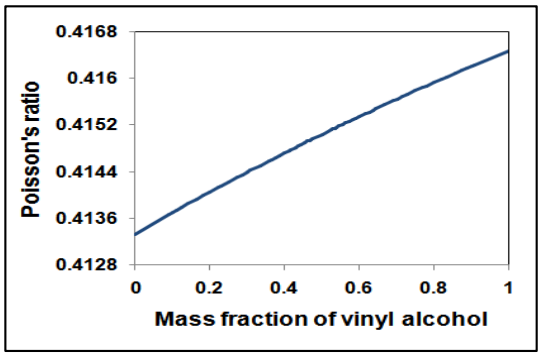

Figure 4. Change in Poisson modulus with mass fraction of poly vinayl alcohol

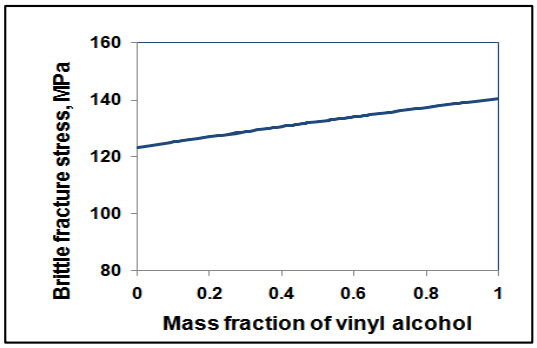

Figure 5. Change in brittle fracture stress with mass fraction of poly polyvinayl alcohol

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Poly (Biphenyl Dimethylcarbonate) and Polydimethylsiloxane (PDMS) Composite

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ABSTRACT

Polymeric blends are useful in preparing hybrid materials with improved properties, related to packaging application. Blends are basically prepared with two or more than two polymers. The improvements in physical and chemical property of these blends are strongly depicted through their molecular level of interactions and therefore, guided by their mixing compatibility or homogeneity of the blends. To get the desired mechanical and gas barrier performance of the prepared poly (biphenyl dimethylcarbonate) (PC) based packaging material, the optimum composition of PC with polydimethylsiloxane (PDMS) was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density was found to increase with the increase in poly (biphenyl dimethylcarbonate) fraction or lowing of polydimethylsiloxane fraction. The permeability properties of the blend were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases decreased with increase in mass fraction of biphenyl dimethyl carbonate. This in-silicostudy helps us to determine the best composition of the blend without performing laboratory experiments which saves valuable time and wastage of raw materials too

Keywords: Gas permeability, Blend, in-silico analysis, Compatibility, Packaging

INTRODUCTION

Polymeric blends are usually offered improved physical and chemical properties like thermal, mechanical, gas barrier and biodegradability [1]. These properties are the prime interest for the researchers to design best packaging material. Gas permeability is sometimes offered as essential criterion to design the polymer for biomedical and industrial utilization. For instance, polymers with high barrier properties, i.e. low permeability, are mandatory for food packaging applications to prevent loss of aroma, color and food-value and to slow down spoilage [2]. Apart

from this food packaging application; there are lots of other applications which require the polymers to have high, low or tailored permeability like, filters and membranes for gas or liquid separation [3], protective coatings (e.g., paints and varnishes) [4], polymer coatings for controlled drug release [5] and water desalination [6].The permeability of liquids and gases through polymer membranes (plastic films) may be happened by either a temperature or pressure gradient, or by concentration gradient or external force field. The ''solution-diffusion'' mechanism is generally used to depict the pathway of gas permeation. It involvesthree steps. In the first step absorption of small molecules is happened into the membrane at the side of higher gradient (concentration, pressure, etc). On the other hand, second step involves the molecular diffusion through the membrane and the final step is related to desorption of those molecules from the membrane at the opposite side of lower gradient. The gas permeability in a polymer is generally varied with the nature of polymer and permeates. It may be accounted due to various degree of crystallinity and porosity of the polymers along with surface functionality (hydrophilic/ hydrophobic groups).

The main aim of combining polymeric materials is to achieve the desired quality of the material. Among various polymers, poly (biphenyl dimethylcarbonate) (PC) is a widely used engineering plastics because of its physical and chemical properties like ductility, good thermal stability, excellent transparency, and high mechanical strength[7]. As a resultof these excellent properties, PC has been largely employed in electronic and electronic appliances along with automotive industry, having an annual production of 6 million tons. Recent report by Behboudiet. al. [8] shows thatPC is blended withpolyvinyl chloride (PVC)to preparethe ultrafiltration membrane for water purification. On the other hand, PC is also blended with poly(vinylidene fluoride) (PVDF) to prepare mechanically strong multicomponent nanocomposites with nanostructural reinforcement of graphenenanoplates, carbon nanotube, and organically modified montmorillonite [9]. In another recent report Wen et al. reinforced the graphene plates into blend of polybutyleneterethalate and polycarbonate [10] to obtain electrical and thermal conductive materials. The unique material, formed from the blend of PC with polystyrene is also reported to sense organic vapours with incorporation of multiwalled carbon nanotubes (MWCNTs) [11]. Polycarbonate blended polysulfone material is recently observed to have improved thermal and mechanical properties[12].

Therefore,investigationof blending compatibility of polycarbonate with other polymer is the urgent need of current research to develop advanced functional materials. All the above mentioned examples relied on laboratory experiments. Usually, preparation of homogeneous blend in wet-lab condition, requires huge time and wastage of materials which can be minimized by in-silico approach through material studio [13] of "Biovia" software. In present context, we are focusing to optimize the homogeneous blend composition of poly (biphrnyl dimethylcarbonate) (PC) with polydimethylsiloxane (PDMS) in terms of gas permeability. Polydimethylsiloxane is a polymeric organosilicon compound, especially known for its unordinary rheological practices. Also it is optically clear, non-harmful and non-combustible. Polydimethylsiloxane (PDMS) shows wide applications like contact focal points, clinical gadgets and advanced elastomer materials. It is likewise utilized in creation of ointments and heat-resistant tiles. As of late, Adreeset. al. [14] prepared the PDMS based mixed layers with polyvinyl chloride-co-vinyl acetic acid derivative (PVCA) for CO_2seperation. Polydimethylsiloxane is likewise utilized in biomedical application like maxillofacial prosthetics, fake veins and articular ligament substitution, when it is mixed with poly (ether) ketone (PEEK) [15]. Consequently, the present in-silico approach towards examination of gas permeability of the blend having various composition of poly (biphenyldimethyl carbonate) (PC) and polydimethylsiloxane (PDMS) might be used to upgrade the sythesis to create attractive advanced materials for packaging applications.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systems of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of poly (biphenyl dimethylcarbonate) and polydimethylsiloxane (PDMS) were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of poly (biphenyl dimethylcarbonate) on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of poly(biphenyl dimethylcarbonate)and polydimethylsiloxaneas potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar Volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite increasedlinearly with increase in mass fraction of biphenyl dimethyl carbonate.

Density: Increase in density indicates decrease in porosity. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite increased linearly with increase in mass fraction of biphenyl dimethyl carbonates. Therefore, prepared materials offered compact structures which may not be suitable for adsorption, but suitable for packaging material, where high gas barrier property is required.

Permeability of Gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium.Lower permeability indicates longer time lag for the gas to pass through the membrane. Figure 3 shows that the permeability of oxygenthrough the hybrid polymer decreased with increase in mass fraction of biphenyl dimethyl carbonate. On the other hand, Figure 4 shows that the permeability of nitrogenthrough the hybrid polymer is decreased with increase in mass fraction of biphenyl dimethyl carbonate. Same pattern is also observed in case of permeability of CO_2 through the hybrid polymer. Figure 5, shows that the permeability of carbon dioxidethrough the hybrid polymer decreased with increase in mass fraction of biphenyl dimethyl carbonate. Thus the results indicated that an increase in biphenyl dimethyl carbonate fraction reduced the permeability of different gases. The rate of permeability might be influence by the molecular weight of the gases.

CONCLUSION

The possibility of use of poly (biphenyl dimethylcarbonate)and polydimethylsiloxaneto form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties.The molar volume and density decreased with increase in biphenyl dimethyl carbonate fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeabilityfor all the gases decreased with increase in mass fraction of

biphenyl dimethyl carbonate. Usually components for a blend are identified experimentally. This in-silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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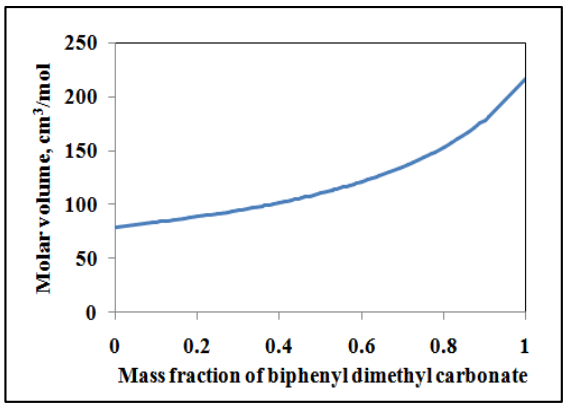

Figure 1. Change in molar volume with mass fraction of biphenyl dimethyl carbonate

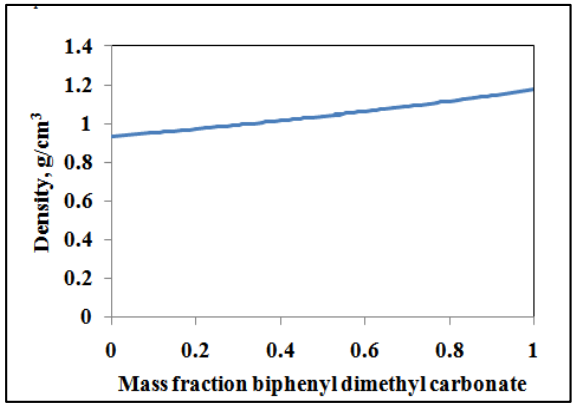

Figure 2. Change in density with mass fraction of biphenyl dimethyl carbonate

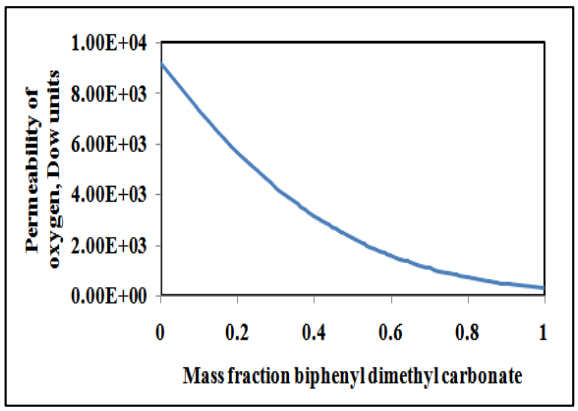

Figure 3. Change in permeability of oxygen with mass fraction of biphenyl dimethyl carbonate

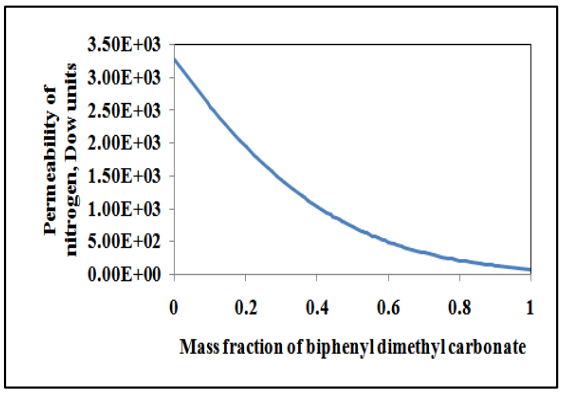

Figure 4. Change in permeability of nitrogen with mass fraction of biphenyl dimethyl carbonate

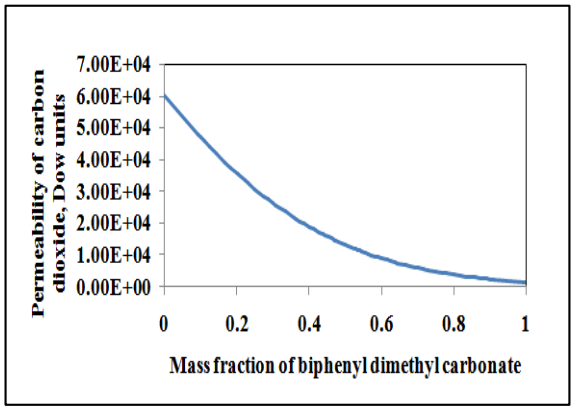

Figure 5. Change in permeability of carbon dioxide with mass fraction of biphenyl dimethyl carbonate

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyacrylic Acid and Poly (1, 2-α -D-Galactose) Composite

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ABSTRACT

Generally, blend is designed with the mixing of two or more components. The change in properties of polyacrylic acid and poly-1, 2-α-D-galactosewas studied in a miscible blend using Biovia Materials Studio. The permeability properties of composition of the blend were studied so that it can be used in different potential application. The molar volume and density of the blend was observed to be decreased with increase in acrylic acid fraction. The gas permeability properties of the composite were observed based on permeability of oxygen, nitrogen and carbon dioxide. From the results, it was noticed that the permeability for all the gases such as oxygen, nitrogen and carbon dioxide are increased with increase in mass fraction of acrylic acid. This technique will be useful us to determine pairs without performing laboratory experiments and also without using materials and money.

Keywords: Blend; Biovia Material Studio; Gas permeability properties; Polyacrylic acid; Insilico analysis

INTRODUCTION

Blends or composites are formed with combination of more than one component where components do retain their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. It is important to develop a single material with the required property for significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Therefore, utilizing blend gives several benefits as it reduces the cost of development of products with required properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material assisted polymer composites and functionalized polymer are used in various environmental applications [1]. Polymers assisted with carbon based (graphene, carbon quantum dot, carbon nano-tube) nano-materialshave drawn special attention towards use in various applications. Researcher has also synthesized natural

fiber based polymer composites to enhance mechanical properties and water resistance [2]. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money.Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Acrylic acid is an organic compound which contains a vinyl group attached to carboxylic acid.It can be used in various purpose such as dispersing agent,artificial teeth and bone repair because of its biocompatibility, biodegradability nature and low toxicity [8-10]. Polyacrylic acid as water soluble polymer have been given as special attention because it can be applied in various applications such as ion exchange, efficient corrosion inhibitor and capacitorsand also it is used for preparing hydrogels. It is not toxic and does not cause irritation [11]. Researchers have used D-galactose in combination with other materials to different applications [12]. Poly-1, 2-α-D-galactose has been reported to be used in Curtius reaction. This study is intended to find out the change of gas permeability value of blend of polyacrylic acid and poly-1, 2-α-D-galactosewith different proportions.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyacrylic acid and poly-1, 2-α-D-galactose werefed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyacrylic acid on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work, the use of polyacrylic acidandpoly-1, 2-α-D-galactoseas potential components of a composite was analyzed using Biovia Materials Studio.Biovia Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar Volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite decreases with increase in mass fraction of acrylic acid.

Density: Increase in density indicates decrease in porosity. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite decreases linearly with increase in mass fraction of acrylic acid.

Permeability of Gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium.Lower permeability indicates longer time lag for the gas to pass through the membrane. Figure 3 shows that the permeability of oxygenthrough the composite increases with increase in mass fraction of acrylic acid.

Figure 4 shows that the permeability of nitrogenthrough the composite increases with increase in mass fraction of acrylic acid. Figure 5 shows that the permeability of carbon dioxidethrough the composite increases with increase in mass fraction of acrylic acid.

CONCLUSION

The gas permeability properties of blend which is formed from polyacrylic acidand poly-1, 2-α-D-galactoseare analyzed using Biovia Materials Studio. The molar volume and density decreased with increase in acrylic acid fraction. The permeability properties of the composite were noticed based on permeability of oxygen, nitrogen and carbon dioxide. From the results, it was observed that the permeabilityfor all the gases increased with increase in mass fraction of acrylic acid. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments without use of chemicals.

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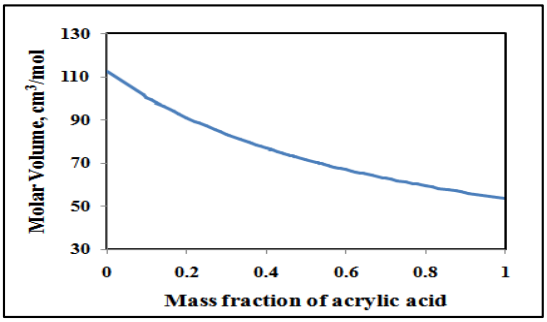

Figure 1. Change in molar volume with mass fraction of acrylic acid.

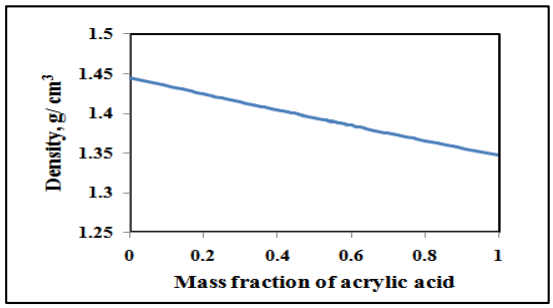

Figure 2. Change in density with mass fraction of acrylic acid

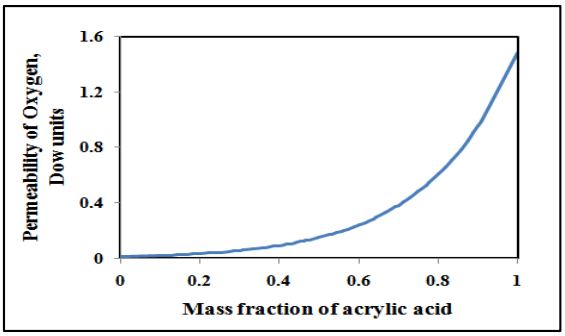

Figure 3. Change in permeability of oxygen with mass fraction of acrylic acid.

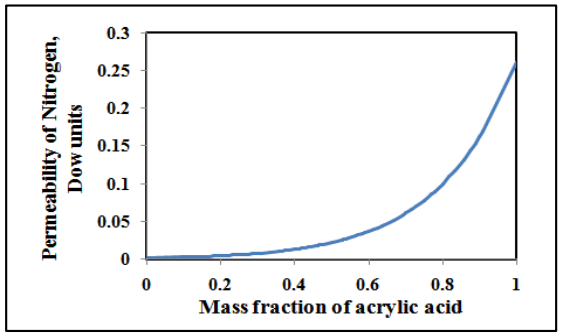

Figure 4. Change in permeability of nitrogen with mass fraction of acrylic acid.

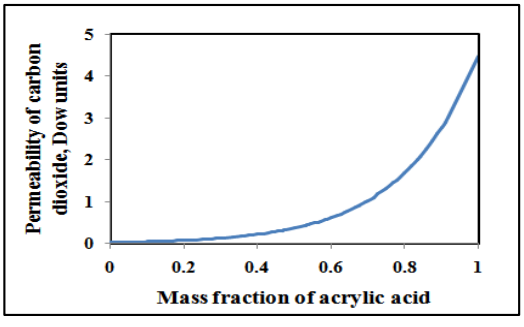

Figure 5. Change in permeability of carbon dioxide with mass fraction of acrylic acid.

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyvinyl Alcohol and Poly-1,2-β-D Galactose Composite

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ABSTRACT

A blend is a mixture of more than one components. The desired property of a blend is its homogeneity. The composition of polyvinyl alcohol and poly-1,2-β-D galactose to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in polyvinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases increase in mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Silico, polyvinyl alcohol, poly-1,2-β-D galactose.

INTRODUCTION

Blends or composites are materials containing more than one components. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of

lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money.Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11].

Researchers have found applications of glycopolymers (synthetic polymers containing pendant carbohydrate groups) in the separation and removal of toxins and bacteria, tumor cell recognition and glucose-responsive insulin delivery [12]. It has been found that biopolymer blends possess good thermal stability [13].This study is intended to identify the interaction of polyvinyl alcohol and poly-1,2-β-D galactose to form composite.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction

Methodology: The structures of polyvinyl alcohol and poly-1,2-β-D galactose were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly-1,2-β-D galactose as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar Volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Density: Increase in density indicates decrease in porosity. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Permeability of Gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium.Lower permeability indicates longer time lag for the gas to pass through the membrane. Figure 3 show that the permeability of oxygenthrough the composite decreases with increase in mass fraction of vinyl alcohol.

Figure 4 shows that the permeability of nitrogen through the composite decreases with increase in mass fraction of vinyl alcohol. Figure 5 shows that the permeability of carbon dioxide through the composite decreases with increase in mass fraction of vinyl alcohol. Thus the results indicated that an increase in vinyl alcohol fraction reduces the permeability of different gases. The rate of permeability might be influence by the molecular weight of the gases.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly-1,2-β-D galactose to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties.The molar volume and density decreased with increase in vinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeabilityfor all the gases decreased with increase in mass fraction of vinyl alcohol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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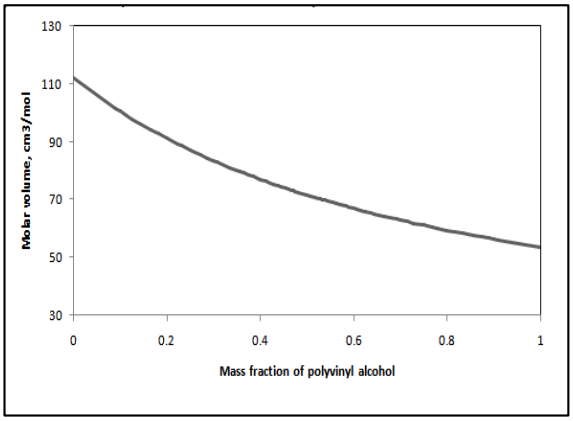

Figure 1. Change in molar volume with mass fraction of vinyl alcohol

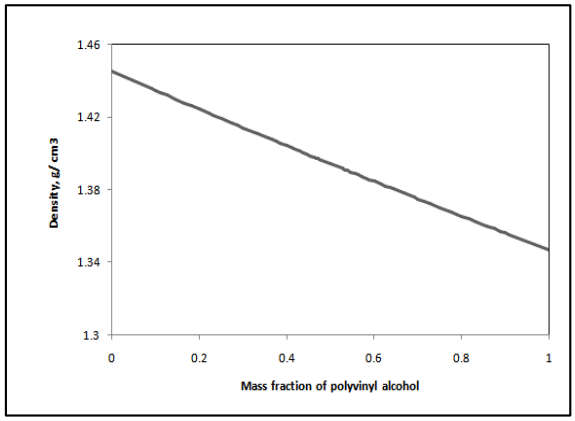

Figure 2. Change in density with mass fraction of vinyl alcohol

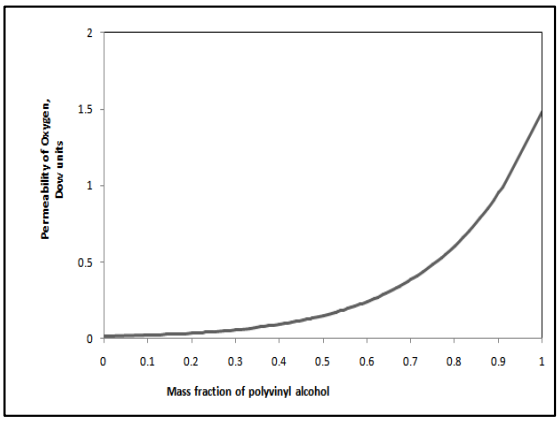

Figure 3. Change in permeability of oxygen with mass fraction of vinyl alcohol

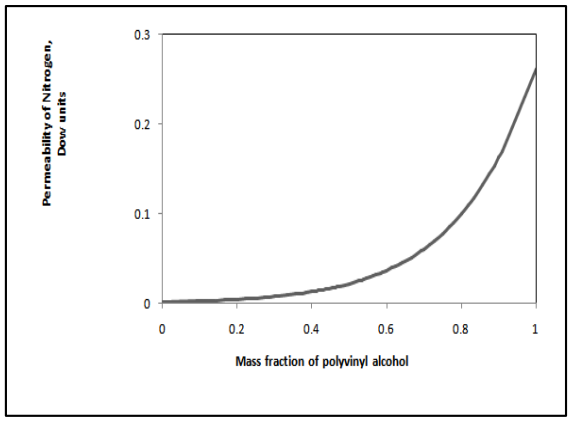

Figure 4. Change in permeability of nitrogen with mass fraction of vinyl alcohol

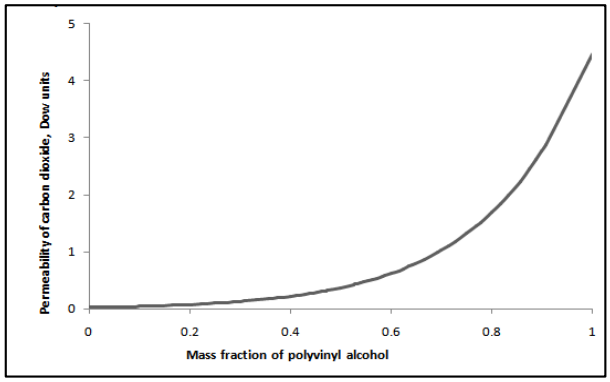

Figure 5. Change in permeability of carbon dioxide with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyvinyl Alcohol and Poly-1, 3-α-D-Galactose Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of polyvinyl alcohol and poly-1,3-α-D-Galactoseto provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density increase in polyvinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases increase in mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Silico, polyvinyl alcohol, Poly-1,3-α-D-Galactose

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of

lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money.Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11]. Researchers have found applications of glycopolymers (synthetic polymers containing pendant carbohydrate groups) in the separation and removal of toxins and bacteria, tumor cell recognition and glucose-responsive insulin delivery [12]. It has been found that biopolymer blends possess good thermal stability [13].This study is intended to identify the interaction of polyvinyl alcohol acid and Poly-1,3-α-D-Galactoseto form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and Poly-1,3-α-D-Galactose were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and Poly-1,3-α-D-Galactoseas potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar Volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Density: Increase in density indicates decrease in porosity. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Permeability of Gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium.Lower permeability indicates longer time lag for the gas to pass through the membrane. Figure 3 shows that the permeability of oxygenthrough the composite decreases with increase in mass fraction of vinyl alcohol. Figure 4 shows that the permeability of nitrogen through the composite decreases with increase in mass fraction of vinyl alcohol. Figure 5 shows that the permeability of carbon dioxide through the composite decreases with increase in mass fraction of vinyl alcohol. Thus the results indicated that an increase in vinyl alcohol fraction reduces the permeability of different gases. The rate of permeability might be influence by the molecular weight of the gases.

CONCLUSION

The possibility of use of polyvinyl alcohol and Poly-1,3-α-D-Galactoseto form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties.The molar volume and density decreased with increase in vinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeabilityfor all the gases decreased with increase in mass fraction of vinyl alcohol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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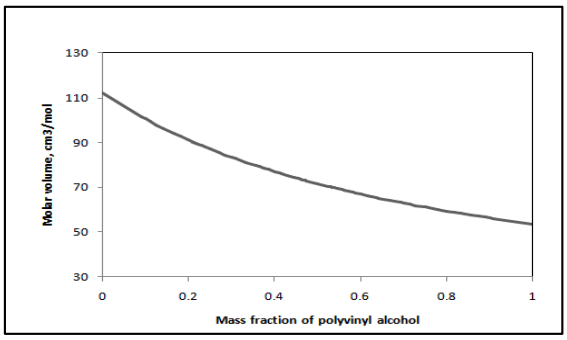

Figure 1. Change in molar volume with mass fraction of vinyl alcohol

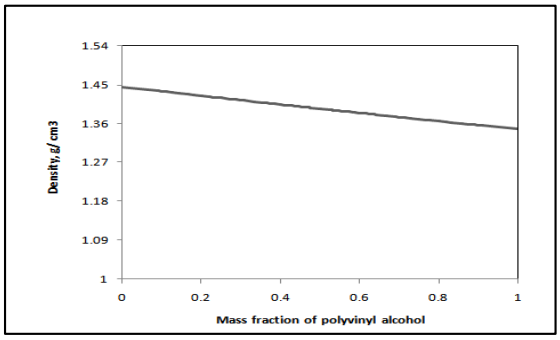

Figure 2. Change in density with mass fraction of vinyl alcohol

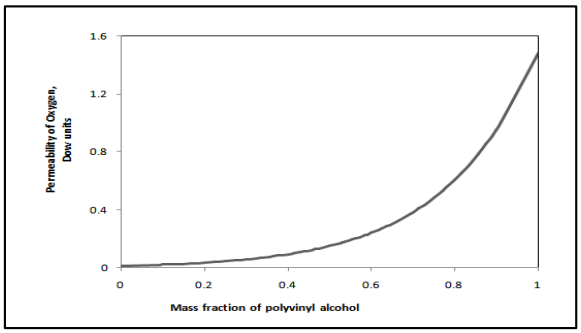

Figure 3. Change in permeability of oxygen with mass fraction of vinyl alcohol

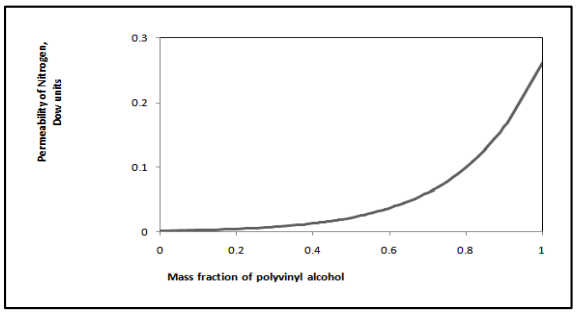

Figure 4. Change in permeability of nitrogen with mass fraction of vinyl alcohol

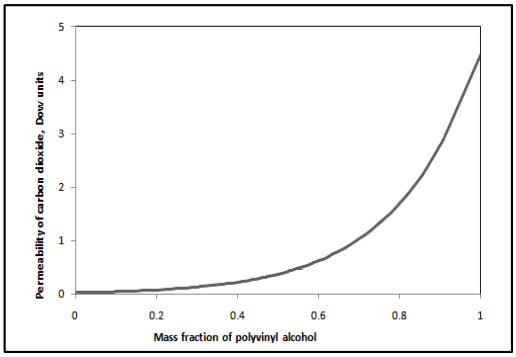

Figure 5. Change in permeability of carbon dioxide with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyvinyl Alcohol and Polyabenzamide Composite

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ABSTRACT

A blend is a mixture of more than one components. The desired property of a blend is its homogeneity. The composition of polyvinyl alcohol and polyabenzamideto provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in polyvinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases decreased with increase in mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: gas permeability properties,Silico, polyvinyl alcohol, polybenzamide.

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The strategy used here for synthesis of poly(benzamide)s relies on polymer end groups being more reactive than the monomer itself resulting in a kinetically controlled living chain-growth polymerization. Because of good control over the polydispersity and the molecular weight, a number of different polymer [12].Polybenzamidehave been reported to be used in Curtius reaction. This study is intended to identify the interaction of polyvinyl alcohol and polybenzamide to form composite.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

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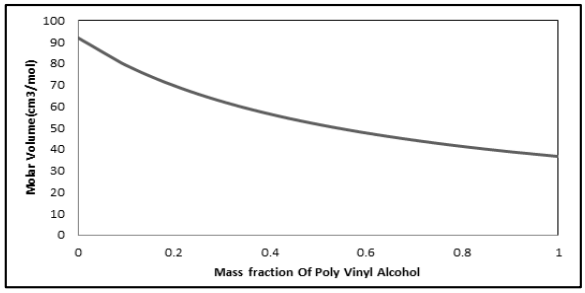


Figure 1. Change in molar volume with mass fraction of vinyl alcohol

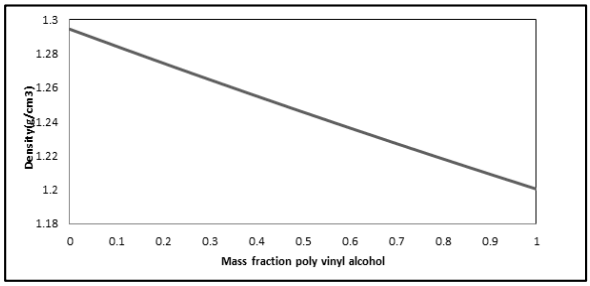


Figure 2. Change in density with mass fraction of vinyl alcohol

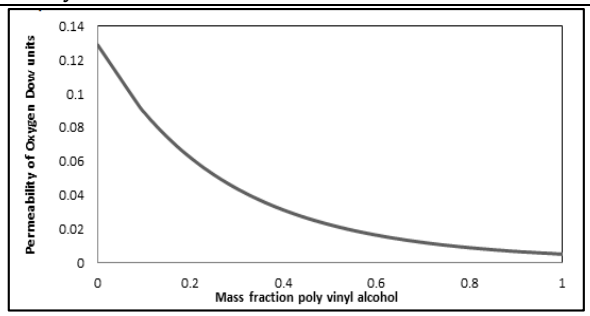


Figure 3. Change in permeability of oxygen with mass fraction of vinyl alcohol

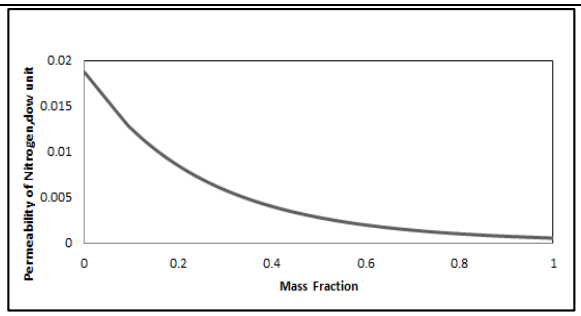
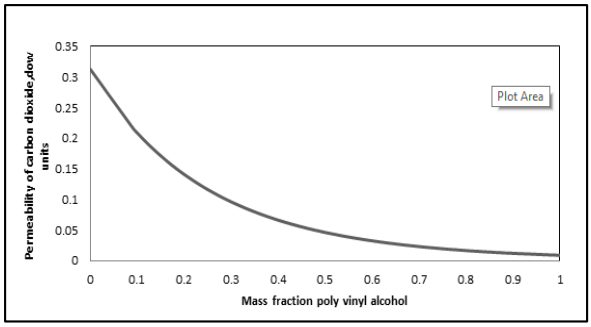


Figure 4. Change in permeability of nitrogen with mass fraction of vinyl alcohol



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RESEARCH ARTICLE

In Silico Analysis of Gas Permeability Properties of Polyvinyl Alcohol and Poly (Biphenyl Dimethyl Carbonate) Composite

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ABSTRACT

Usually, blend is a mixture of two or more components and expected to have homogeneity. In this paper, we have tried to explore the compatibility of polyvinyl alcohol and poly(biphenyl dimethyl carbonate) to form a miscible blend using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in polyvinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases decreased with increase in mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Gas Permeability Properties, Polyvinyl Alcohol, Biphenyl Dimethyl Carbonate.

INTRODUCTION

Blends or composites are materials containing more than one components. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of

transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money.Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.

Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11]. Poly(biphenyl dimethyl carbonate) has an amorphous structure and is considered to be an engeeniering plastic. Its wide applications include impact resistance, strength, high temperature performance, toughness, load bearing capabilities, dimensional stability, flame retarding capabilities, and excellent optical clarity. Based on these properties they have commercialized as outdoor signs, eye glasses, compact disks, CD-ROM, aircraft windows, automotive windows and instrument panels, food trays and containers, automotive headlamp covers, housings of appliances, and medical devices [12, 13]. It has been found that biopolymer blends possess good thermal stability [14]. This study is intended to explore the gas permeability properties of the blends developed by varying the mass fraction of polyvinyl alcohol and poly(biphenyl dimethyl carbonate) using synthia.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and poly(biphenyl dimethyl carbonate) were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly (biphenyl dimethyl carbonate) as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar volume: It is the volume occupied by one mole of a substance. Figure 1 shows that the molar volume of the composite decreases with increase in mass fraction of vinyl alcohol.

Density: Increase in density indicates decrease in porosity. A higher porosity will enhance the surface area making in suitable for absorption/adsorption applications. Figure 2 shows that the density of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Permeability of gas: Permeability is the rate at which the gas can pass through the polymer membrane after the gas has come to equilibrium.Lower permeability indicates longer time lag for the gas to pass through the mebrane. Figure 3 shows that the permeability of oxygenthrough the composite decreases suddenly with increase in mass fraction of vinyl alcohol. Thus the results indicated that an increase in vinyl alcohol fraction reduces the permeability of different gases. The rate of permeability might be influence by the molecular weight of the gases.

CONCLUSION

The possibility of use of polyvinyl alcohol and andpoly(biphenyl dimethyl carbonate) to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties.The molar volume decreased and density increased with increase in vinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeabilityfor all the gases decreased tremendously with increase in mass fraction of vinyl alcohol. This indicates that these blends with high polyvinyl mass fraction can be used as good packaging materials. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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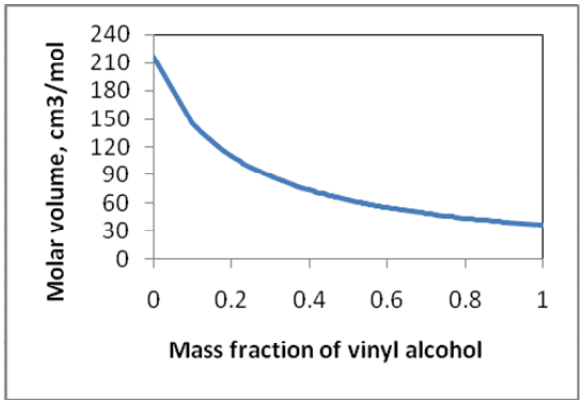

Figure 1. Change in molar volume with mass fraction of vinyl alcohol

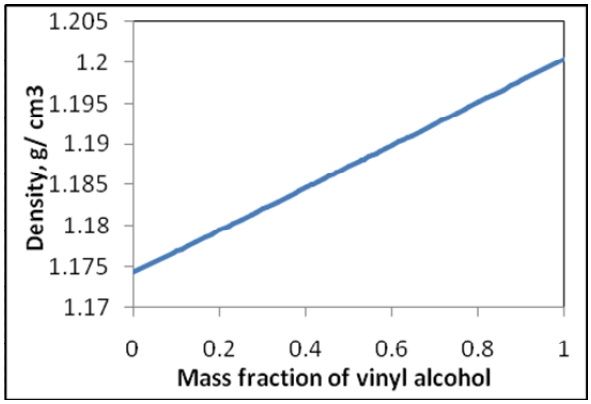

Figure 2. Change in density with mass fraction of vinyl alcohol

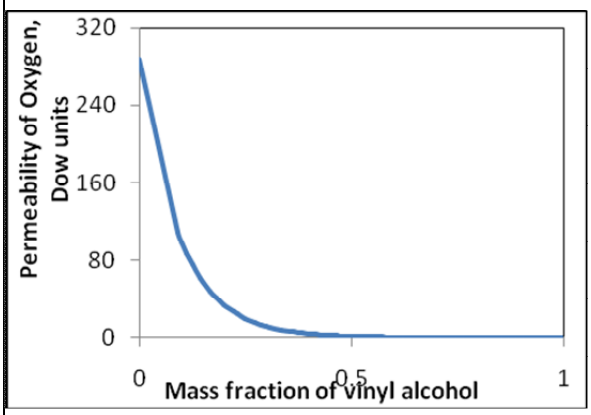

Figure 3. Change in permeability of oxygen with mass fraction of vinyl alcohol

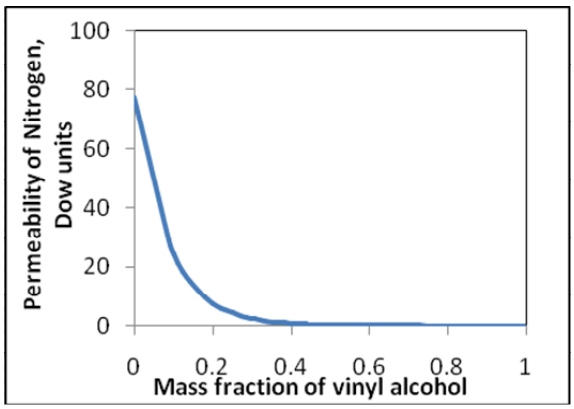

Figure 4. Change in permeability of nitrogen with mass fraction of vinyl alcohol

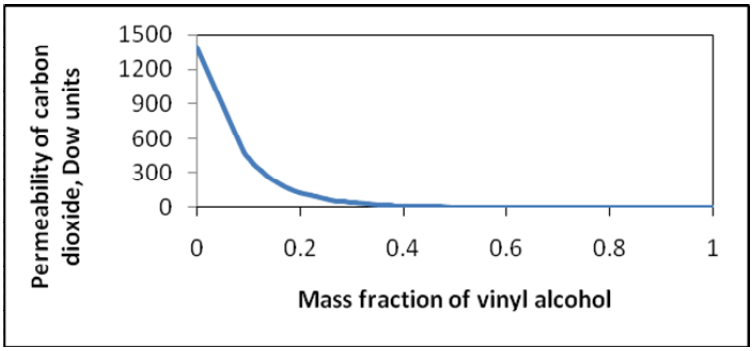

Figure 5. Change in permeability of carbon dioxide with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Polyvinyl Alcohol and Poly Ethylene Terephthalate Composite

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ABSTRACT

A blend is created bythe combination of two or more components. The compatibility of polyvinyl alcohol andpoly ethylene Terephthalate was study to form a miscible blend using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in polyvinyl alcohol fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide.The results showed that the permeability for all the gases decreases with increase in mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Synthia; In silico; Polyvinyl alcohol; Polyethylene terephthalate; Gas permeability

INTRODUCTION

Blends or composites to be formed with combination of more than one component where components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisable to mix dissimilar components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilize the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of improvement of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material customized polymers paved the way to multi useful materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire evidence materials [3]. There are reports of inorganic additives in polypropylene; that can

enhance flame retardancy lacking increasing the weight [4]. Researchers have emphasize on synthesis and production of lightweight composite material having high strength important for enhancing fuel efficiency in the field of transport [5]. There are application of composites in structural Engineering due to high strength to weight ratio and resistance to decay. Thus, glass fiber durable polymers, latex polymer cementitious composites [6] were developed for building of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mention example relied on laboratory experiments. Usually blends are prepared by test and fault method andthis method is a low cost and less time consuming method. Thus, researchers have focused on the use of in silico move toward to develop new blends. Software (Materials Studio [7]) has been used to identify well-matched pairs. Among the a mixture of polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, simple film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is extensively used in covering industry to form strong polymeric films. It is because of their high mechanical power, environmental stability and easy processability [10]. On the other hand, PVA is poisonous, semicrystalline, hydrophilic, biocompatible and simply soluble in water [11].

The consumption of plastics in Western Europe is of 38 million tonnes per year, the majority of which are used in the production of plastic packaging, household and domestic products, electrical and electronic goods [12]. There is also significant consumption of plastics for the structure and construction industry and automotive industry. The two main types of plastics are thermoplastics, which soften when heated and harden again when cooled, and thermosets, which harden by curing and cannot be re-moulded. About 80 % of plastics used in Western Europe are thermoplastics [13].For many waste landfills is the largest route for disposal throughout the countries of Europe. For some countries, including Lithuania, more than 60 % of municipal solid waste is disposed of to landfill [14]. Plastics make up high proportion of waste that volume and range used increases dramatically. Although plastics make up between 5 wt.% and 15 wt.% of municipal solid waste it comprises 20 % – 30 % of the volume [13]. Most plastics are non-degradable and take a long time to decompose, possibly up to hundreds of years – although no-one knows for certain as plastics have not existed for long enough, when they are landfilled. It is estimated that only about 50 % of the plastics produced in Western Europe each year are available for collection and recycling [12 – 14]. According to the experts from Kaunas University of Technology in Lithuania plastics reach about 82 thousands tones of municipal solid waste in 2004. It comprised about 24 kg for one inhabitant [15]. Waste recycling in Lithuania increases constantly andduring 2000–2006 it ranges between 20 – 35 thousand tonnes per year [16]. According to the Environmental Protection Agency (EPA) "recycling" is considered to be processing of waste to make new article. There are divided three distinct approaches to the recycling of post-consumer plastic materials :1) it could be reused directly; 2) undergo physical reprocessing, for example, grinding, melting and reforming; 3) be subjected to chemical treatment, when components are isolated and reprocessed for use in manufacture. A new widespread nomenclature of recycling was adopted by EPA. Primary recycling involves the use of pre-consumer industrial scrap and salvage, while physical reprocessing refers as secondary recycling and chemical processing as tertiary recycle [16].

MATERIALS AND METHODS

Software Used: Equipment studio part of Biovia software (Dassault Systemes of France) was used for analysis. The software utilize machine study techniques and normal algorithms to predict the level of interaction.

Methodology: The structure of polyvinyl alcohol andpoly ethylene Terephthalatewere fed to the synthia menu of equipment Studio. It was then run for different weight fractions of the mechanism. Different property of the composite was displayed in a tabular form. The values to be used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the gass properties of the composite.

RESULTS AND DISCUSSION

The use of polyvinyl alcohol andpoly ethylene Terephthalate as potential mechanism of a composite was analyze using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-define correlation (advanced quantitative structure-property relationships) to estimate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. accordingly, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic relations that give rise to it. However, the main shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculate.To overcome this limitation, the technique implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from diagram theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar Volume: The molar volume occupied by one mole of a substance at given at a given temperature and pressure.Figure 1 shows that the molar size of the composite decrease linearly with rise in dimension small part of mass fraction of polyvinyal alcohol.

Density: The density in increase indicates drop in porosity. A advance porosity will enhance the float up part creation in apposite for absorption application. Figure 2 shows that the density of the composite decrease linearly with incrase in mass fraction of polyvinayl alcohol.

Permeability of Gas: Permeability is the rate by which the gas can pass through the polymer membrane following the gas has come to equilibrium. Lower permeability indicate longer time lag for the gas to pass through the membrane. Figure 3 shows that the permeability of oxygen through the composite decreases with increase in mass division of polyvinyl alcohol.

Figure 4 shows that the permeability of nitrogen through the composite decrease with increase in mass fraction of polyvinyl alcohol. Figure-5 shows that the permeability of carbon dioxide through composite decrease with increases of mass fraction poly acrylic acid. As a consequence the domino effect indicated that an multiply in polyvinayl alcohol reduces the permeability capacity be weight by the molecular import of the gases.

CONCLUSION

Possibility of use poly acrylic acid and poly oxyethylene to form a homogeneous blend was explore using Biovia equipment Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in poly acrylic acid. The permeability property of the composite was studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeability for all the gases decreased with increase in mass fraction of vinyl alcohol. Usually components for a blend are recognized experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving equipment, currency and time.

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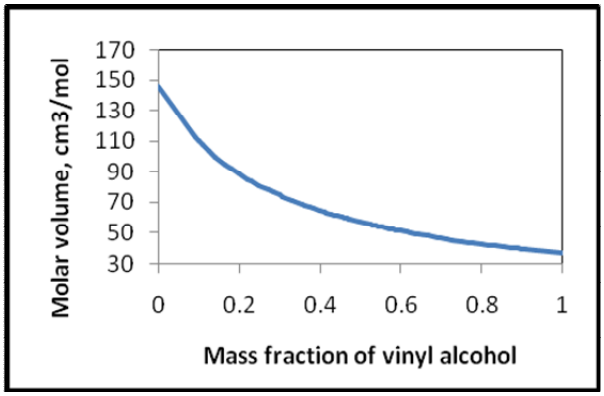

Figure 1. Change in molar volume with mass fraction of poly acrylic acid

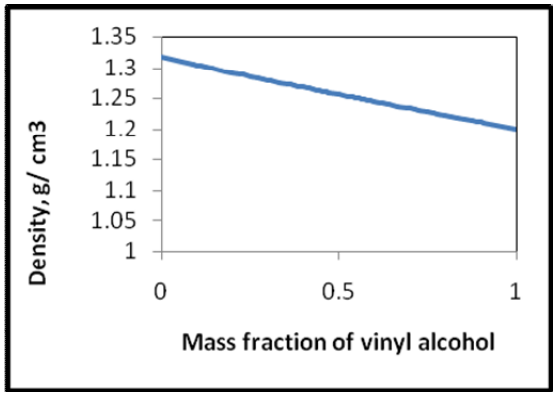

Figure 2. Change in density with mass fraction of polyacrylic acid

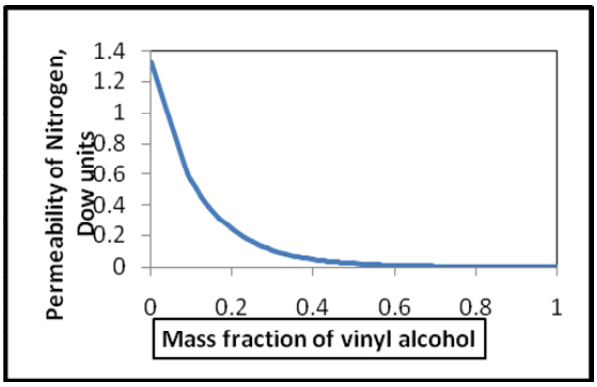

Figure 3. Change in permeability of oxygen with mass fraction of poly acrylic acid

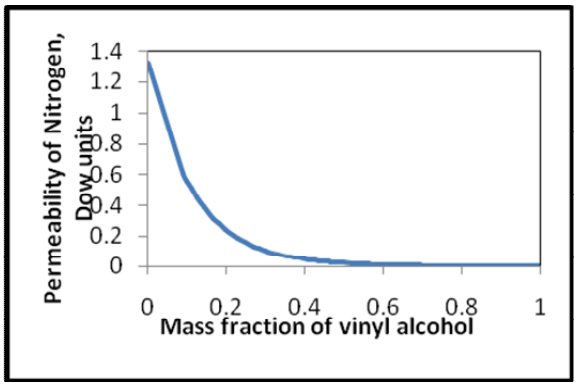

Figure 4. Change in permeability of nitrogen with mass fraction of poly acrylic acid

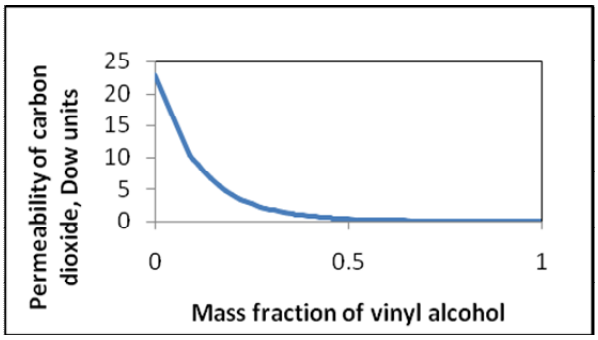

Figure 5. Change in permeability of carbon dioxide with mass fraction of polyvinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyacrylic Acid and Polyoxyethylene Composite

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ABSTRACT

A blend is a combination of additional than one components. The preferred property of a blend is its homogeneity. The composition of poly acrylic acid and poly oxyethylene to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The mechanical properties of the composite to be studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The consequences indicated that the values of all the properties increased with increase in mass fraction of vinyl alcohol.This study will help determine pairs without performing laboratory experiments saving materials, currency and time

Keywords: Synthia; In silico;Polyacrylic Acid;Polyoxyethylene, Mechanical Properties

INTRODUCTION

Blends or composite are resources containing more than one part. The components do retain their identity in the combination. As it is very difficult to find multiple properties in a single material, it is advisableto combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilize the advantages of different materials; mix them to get the preferred property. Thus a blend saves time to develop a new material thereby dipping the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn significant attention in recent years. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized

on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money.Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs. Acrylic acid have a board varity of application in dentistry as denture bases, artificial teeth , denture repair material, maxillofacial appliances for skeletal defects etc.[8] , bone repair [9] dispersing agent, superabsorbent polymer ion replace resin,etc. [10] Polyacrylic acid is a polyelectrolyte soluble in aqueous media at impartial pH It is used for prepare hydrogels. It is not poisonous and does not reason irritation [11].

The area of high pressure molecular credence polymers deliberate were poly (oxythylene) homopolymers (polyox) with molecular with molecular credence ranging from 4,000,000 to 7,000,000 power characteristics optional fine flowability for these resources and predicted case fulfil importance uniformity irritation[12]. Experiments showed a precise extreme notch of bulge for these resources in equality gastric and shock absorber solution[13]. These polymers bottle sustain the discharge percentage of mutually water-soluble and indecipherable drugs from drug providing system. The soothing molecular burden polymers control a fewer marked sustained-release provoke compare to the eminent molecular authority polymer data (i.e individual with 7,000,000 molecular weight). Intensification in the freedom percentage of the drug. The solubility of the drugs openly influenced the make available rate. Discharge kinetics were evaluated and appeared to be influenced by the molecular import of the polymer, the solubility of medicine, and the ratio of the drug to the polymer in the capsule[14]. Biomodal issue kinetics was exhibit by a amount of furosemide formulation (i.e. F5and F8).

MATERIALS AND METHODS

Software Used: Equipment studio module of Biovia software (Dassaults system of france) was old for analysis. The software utilizes piece of equipment education techniques and usual algorithems to predict the degree of interaction.

Methodology: Polyacrylic acid and oxyethelene were prepared by the synthia menu resources studio. It was subsequently enclose for characteristic weight fraction of the components. Varied properties of the composite were displayed in a tabular form. The ethics were second-hand to plot graphs to make out the impression of result little bit of poly-acryalic acid on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of poly acrylic acid and poly oxyethylenes as potential components of a composite was analyzed using Biovia equipment Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to calculate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group involvement cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of

group contributions is required and properties may be predicted for any polymer composed of any mixture of the subsequent The mechanical properties of the composite were premeditated based on size module, Bulk modules, Youngs modulus, Poission ratio and brittle stress fracture.

Bulk Modulus: The Bulk modulus of a substance is a measure of how resistance to compression that substance is. It is defined as the ratio of the infinitesimal pressure increase to the resulting relative to decrease of the volume. Figure 1 shows that the form modulus of the composite increase linearly with fuel in main part of acrylic acid.

Shear Modulus: The shear modulus is defined as the ratio of shear stress to shear strain. It is also known as modulus of rigidity. Figure 2 says that the modulus of rigidity of the composite increase with increase in mass fraction of poly acrylic acid.

Youngs Modulus: Young modulus, is a mechanical property that measures the stiffness of a solid material Figure 3 shows that the Youngs modulus of the composite increase with increase in mass fraction of poly acrylic acid.

Poisson Ratio: Poissons ratio is the ratio of transverse contraction strain to longitudinal extension strain in the direction of stretching force. Figure 4 shows that the poisson ratio of the composite decrease linearly with increase in mass fraction of acrylic acid.

Brittle Fracture Stress: A brittle fracture is the fracture of a metallic object or other material with appreciable prior plastic deformation. It is a break in a brittle piece of metal that failed because stress exceeded cohesion. Figure 5 shows that the brittle fracture stress of the composite decrease in increase in mass fraction of poly acrylic acid.

CONCLUSION

Possibility of use of the poly acrylic acid and poly oxyethylene to form a homogeneous blend was explored using BioviaMaterial Studio. The composition of the blend tobe analyzed with respect to mechanical properties. The mechanical properties of the composite to be studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of two properties decrease with increase mass fractionand the other properties increased with increase in mass fraction of poly acrylic acid. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, currency and time.

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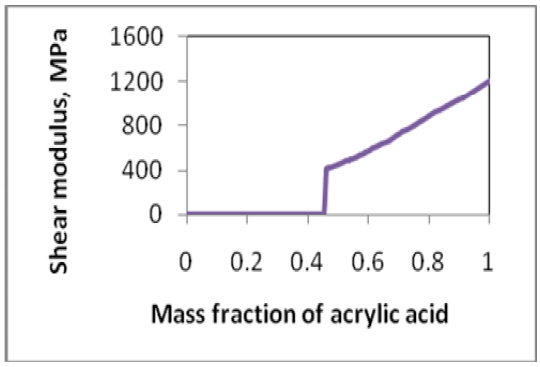

Figure 1. Change in bulk modulus with mass fraction of acrylic acid.

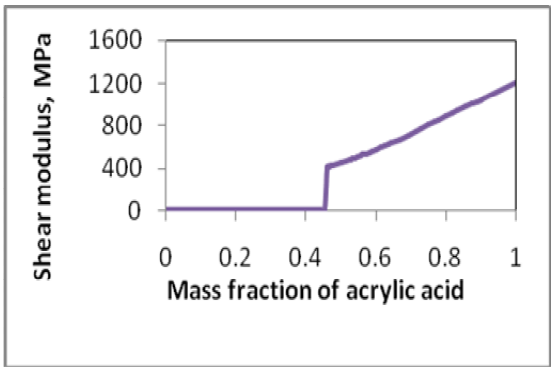

Figure 2. Change in shear modulus with mass fraction of acrylic acid

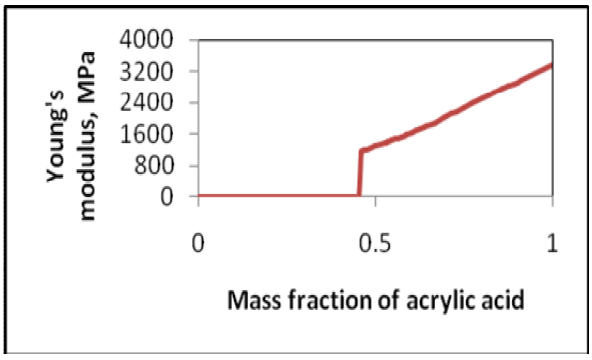

Figure 3. Change in Young's modulus with mass fraction of acrylic acid

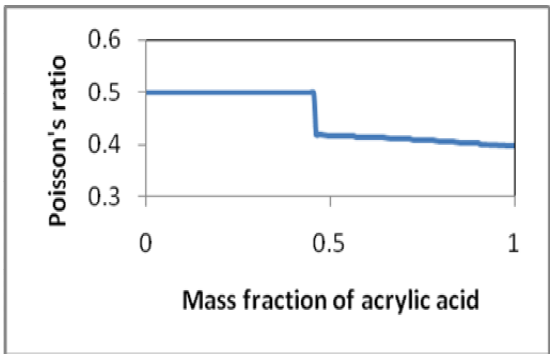

Figure 4. Change in Poisson modulus with mass fraction of acrylic acid.

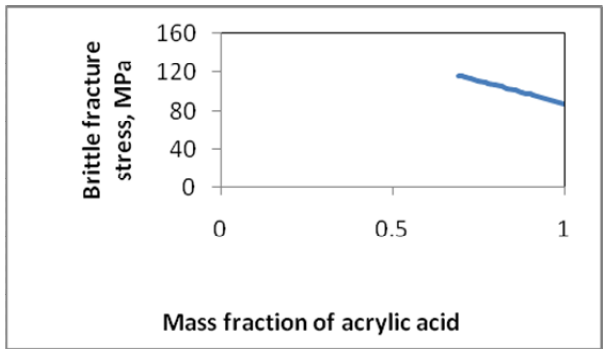

Figure 5. Change in brittle fracture stress with mass fraction of poly acrylic acid

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyvinyl Alcohol and Poly-1, 2-α-D-Galactose Composite

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ABSTRACT

A blend is formed from the combination of two or more components. The change in properties of polyvinyl alcohol and poly-1, 2-α-D-galactosewas noticed to form a miscible blend using Biovia Materials Studio. The composition of polyvinyl alcohol and poly-1, 2-α-D-galactoseto provides desired mechanical properties of the blend were explored using Biovia Materials Studio. The mechanical properties of the blend were studied with considering the bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. From the results, it was noticed that the values of bulk modulus, shear modulus, Young' modulus decreased with increase in mass fraction of vinyl alcohol how ever the values of Poisson ratio and brittle stress fracture modulus increased with increase in mass fraction of vinyl alcohol. This study will help to determine pairs without doing laboratory experiments so that there is no use of materials and it is low cost.

Keywords: Blend; Biovia Material Studio; Mechanical properties; Polyvinyl alcohol; In sillico

INTRODUCTION

Blends or composites are formed from mixing of more than one component where components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisable to combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi-functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber

composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method and this technique is a low cost and less time consuming method. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs. With considering various polymers, polyvinyl alcohol (PVA) is a encouraging material due to its high dielectric strength, easy film formation, adhesiveness and these properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy process ability [10]. On the other hand, PVA is non-toxic, semi-crystalline, biocompatible, hydrophilic and easily soluble in water [11]. There are different applications of glycol polymers (synthetic polymers containing pendant carbohydrate groups) in the separation and removal of toxins and bacteria, tumor cell recognition and glucose-responsive insulin delivery which is reported in earlier literatures[12]. It has been found that biopolymer blends possess good thermal stability [13]. This study is intended to study of mechanical properties of blend of polyvinyl alcohol and poly-1, 2-α-D-galactose.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and poly-1, 2-α-D-galactose werefed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly-1, 2-α-D-galactoseas potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated. To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Bulk Modulus: Bulk modulus is the measure of the decrease in volume with an increase in pressure. Figure 1 shows that the bulk modulus of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Shear Modulus: It is defined as the ratio of shear stress and shear strain. It shows the response of the composite to shear deformation. Figure 2 shows that the shear modulus of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Young's Modulus: It is defined as the ratio of stress and strain. It compares the relative stiffness of the composite. Figure 3 shows that the Young's modulus of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Poisson Ratio: It is the ratio of lateral strain to longitudinal strain. Figure 4 shows that the Poisson ratio of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Brittle Fracture Stress: Brittle Fracture is the sudden, rapid cracking of a material under stress where the material exhibited practically no evidence of ductility or plastic degradation before the fracture occurs. Figure 5 shows that the brittle fracture stress of the composite increases linearly with increase in mass fraction of vinyl alcohol.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly-1, 2-α-D-galactose to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to mechanical properties. The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of Poisson ratio and brittle stress fracture increased with increase in mass fraction of vinyl alcohol. However, the values of bulk modulus, shear modulus and Young' modulus decreased with increase in mass fraction of vinyl alcohol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments so that there is no use of chemicals.

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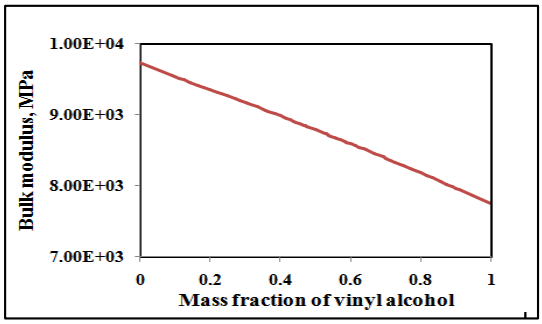

Figure 1. Change in bulk modulus with mass fraction of vinyl alcohol.

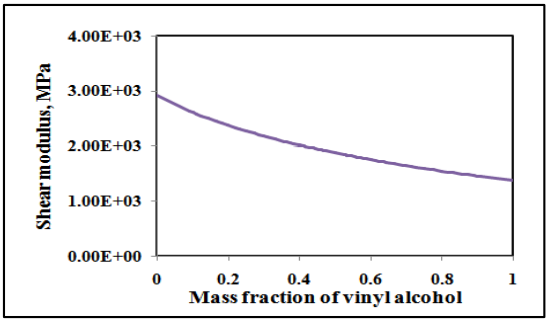

Figure 2. Change in shear modulus with mass fraction of vinyl alcohol

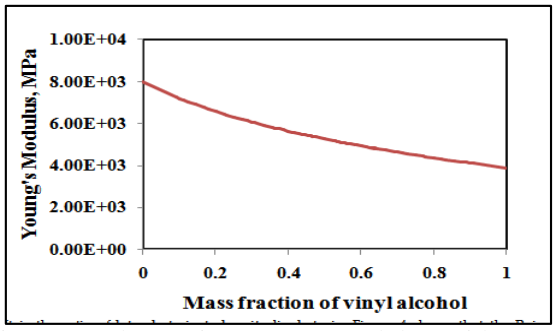

Figure 3. Change in Young's modulus with mass fraction of vinyl alcohol.

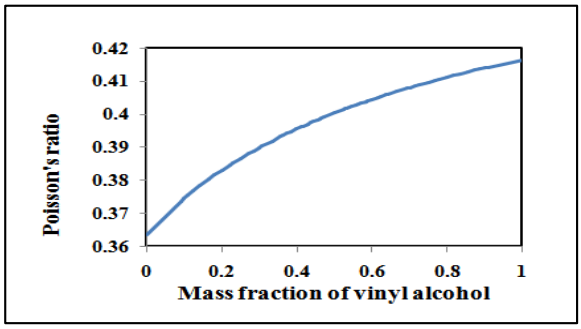

Figure 4. Change in Poisson modulus with mass fraction of vinyl alcohol.

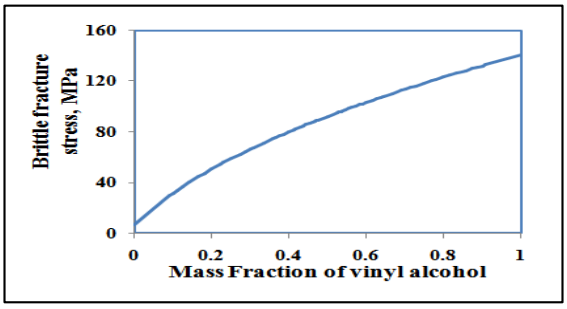

Figure 5. Change in brittle fracture stress with mass fraction of vinyl alcohol.

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyacrylic Acid and Poly (1, 2-α-D-Galactose) Composite

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ABSTRACT

Polymer blend, combination of two or more component, has become the commercial importance due to its different properties of synergistic mixture. The study of physical and mechanical properties of the blend gives the opportunity for solving of different research problems. The mechanical properties of the blend using polyacrylic acid and poly-1, 2-α-D-galactose wereanalyzed using Biovia Materials Studio. The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of Poisson ratio and brittle stress fracture increased with increase in mass fraction of acrylic acid where as the values of bulk modulus, shear modulus and Young' modulus decreased with increase in mass fraction of acrylic acid. Since this technique does not require any chemical and money therefore it is very useful.

Keywords: Blend; Biovia Material Studio; Mechanical properties; Polyacrylic acid; In silico analysis

INTRODUCTION

Polymer blend, containing two or more component, has become the commercial importance due to its different properties of synergistic mixture and these properties are not associated with sum of properties of components. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

In earlier literature, nanomaterial decorated polymer composites have been designed for various applications such as dye removal, sensing, catalyst and packaging [1] and also carbon based nanomaterial assisted with polymers have been used in different environmental applications. Scientist has also synthesized natural fiber based polymer composites to enhance mechanical properties and water resistance [2]. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy

without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method and this technique is a low cost and less time consuming method. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs.

Acrylic acid is an organic compound which contains a vinyl group attached to carboxylic acid.It can be used in various purposes such as dispersing agent,artificial teeth and bone repair because of its biocompatibility, biodegradability nature and low toxicity [8-10]. Polyacrylic acid as water soluble polymer have been given as special attention because it can be applied in various applications such as ion exchange, efficient corrosion inhibitor and capacitorsand also it is used for preparing hydrogels [11]. It is not toxic and does not cause irritation. Researchers have used D-galactose in combination with other materials to different applications [12]. Poly-1, 2-α-D-galactose has been reported to be used in Curtius reaction. This study is intended to find out the change of gas permeability value of blend of polyacrylic acid and poly-1, 2-α-D-galactose with different proportions.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyacrylic acid and poly-1, 2-α-D-galactose were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyacrylic acidon the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acidand poly-1, 2-α-D-galactose as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Bulk Modulus: Bulk modulus is the measure of the decrease in volume with an increase in pressure. Figure 1 shows that the bulk modulus of the composite decreases linearly with increase in mass fraction of acrylic acid.

Shear Modulus: It is defined as the ratio of shear stress and shear strain. It shows the response of the composite to shear deformation. Figure 2 shows that the shear modulus of the composite decreases linearly with increase in mass fraction of acrylic acid.

Young's Modulus: It is defined as the ratio of stress and strain. It compares the relative stiffness of the composite. Figure 3 shows that the Young's modulus of the composite decreases linearly with increase in mass fraction of acrylic acid.

Poisson Ratio: It is the ratio of lateral strain to longitudinal strain. Figure 4 shows that the Poisson ratio of the composite increases linearly with increase in mass fraction of acrylic acid.

Brittle Fracture Stress: Brittle Fracture is the sudden, rapid cracking of a material under stress where the material exhibited practically no evidence of ductility or plastic degradation before the fracture occurs. Figure 5 shows that the brittle fracture stress of the composite increases with increase in mass fraction of acrylic acid.

CONCLUSION

The study of physical and mechanical properties of the blend gives the opportunity for solving of different research problems. The mechanical properties of polyacrylic acid and poly-1, 2-α-D-galactose was studied using Biovia Materials Studio for further use in various applications. The composition of the blend was analyzed with respect to mechanical properties. The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of Poisson ratio and brittle stress fracture increased with increase in mass fraction of acrylic acid where as the values of bulk modulus, shear modulus and Young' modulus decreased with increase in mass fraction of acrylic acid.Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments

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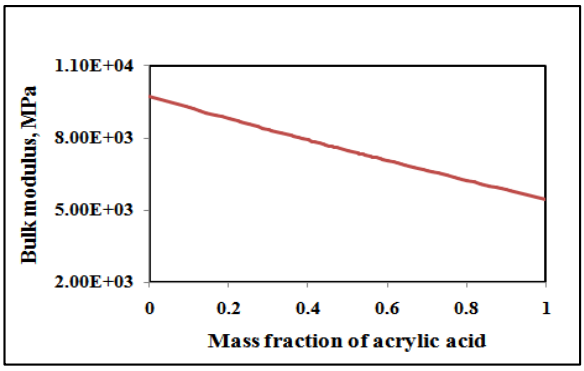

Figure 1. Change in bulk modulus with mass fraction of acrylic acid.

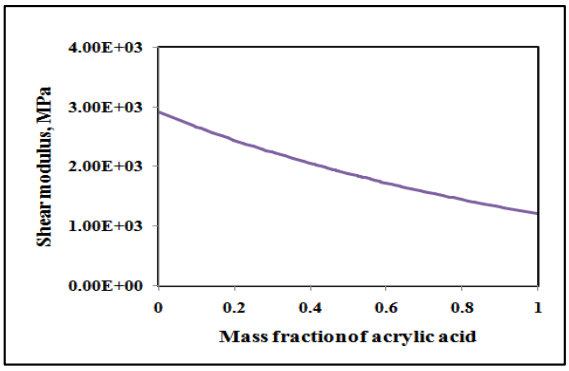

Figure 2. Change in shear modulus with mass fraction of acrylic acid.

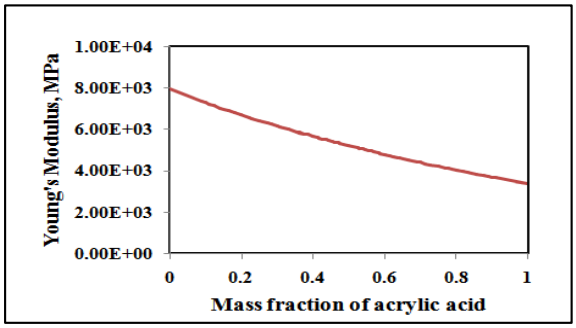

Figure 3. Change in Young's modulus with mass fraction of acrylic acid.

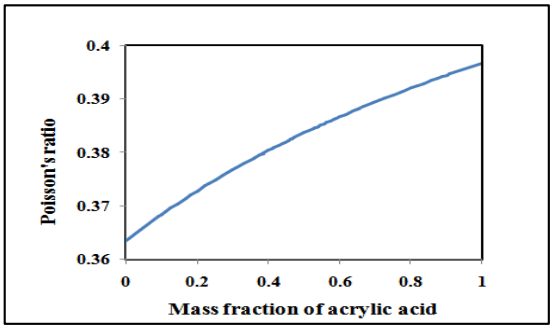

Figure 4. Change in Poisson modulus with mass fraction of acrylic acid.

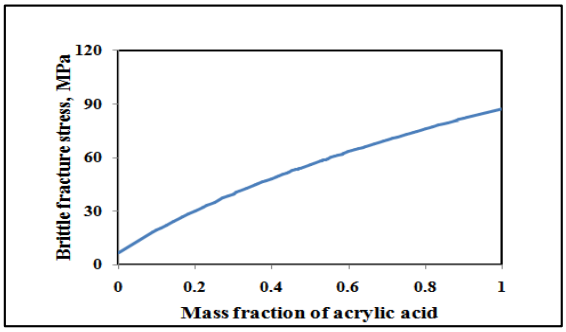

Figure 5. Change in brittle fracture stress with mass fraction of acrylic acid.

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polybiphenyl Dimethyl Carbonate (PC) and Polyether Sulfone Composite

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ABSTRACT

Hybrid polymeric materials with improved mechanical properties are in huge demand in connection to the industrial background. Blending is the simple technique to mixing different polymers and therefore, generating advanced functional materials. The composition of poly (biphenyl dimethylcarbonate) (PC) and polyether sulfone to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The mechanical properties of the composite were studied in terms of bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties decreased with increase in mass fraction of biphenyl dimethyl carbonate.This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Polymer blend, Mechanical properties, Biovia, In-silico analysis, Compatibility

INTRODUCTION

Polymeric blends are usually offered improved physical and chemical properties like thermal, mechanical, gas barrier and biodegradability [1]. These properties are the prime interest for the researchers to design best packaging material. Gas permeability is sometimes offered as essential criterion to design the polymer for biomedical and industrial utilization. For instance, polymers with high barrier properties, i.e. low permeability, are mandatory for food packaging applications to prevent loss of aroma, color and food-value and to slow down spoilage [2]. Apart from this food packaging application; there are lots of other applications which require the polymers to have high, low or tailored permeability like, filters and membranes for gas or liquid separation [3], protective coatings (e.g., paints and varnishes) [4], polymer coatings for controlled drug release [5] and water desalination [6].The permeability of liquids and gases through polymer membranes (plastic films) may be happened by either a temperature or pressure gradient, or by concentration gradient or external force field. The ''solution-diffusion'' mechanism is generally used to depict the pathway of gas permeation. It involvesthree steps. In the first step

absorption of small molecules is happened into the membrane at the side of higher gradient (concentration, pressure, etc). On the other hand, second step involves the molecular diffusion through the membrane and the final step is related to desorption of those molecules from the membrane at the opposite side of lower gradient. The gas permeability in a polymer is generally varied with the nature of polymer and permeates. It may be accounted due to various degree of crystallinity and porosity of the polymers along with surface functionality (hydrophilic/ hydrophobic groups).The main aim of combining polymeric materials is to achieve the desired quality of the material. Among various polymers, polybiphenyldimethylcarbonate (PC) is a widely used engineering plastics because of its physical and chemical properties like ductility, good thermal stability, excellent transparency, and high mechanical strength[7]. As a resultof these excellent properties, PC has been largely employed in electronic and electronic appliances along with automotive industry, having an annual production of 6 million tons. Recent report by Behboudi *et.al.* [8] shows thatPC is blended withpolyvinyl chloride (PVC)to preparethe ultrafiltration membrane for water purification. On the other hand, PC is also blended with poly(vinylidene fluoride) (PVDF) to prepare mechanically strong multicomponent nanocomposites with nanostructural reinforcement of graphenenanoplates, carbon nanotube, and organically modified montmorillonite [9]. In another recent report Wen et al. reinforced the graphene plates into blend of polybutyleneterethalate and polycarbonate [10] to obtain electrical and thermal conductive materials. The unique material, formed from the blend of PC with polystyrene is also reported to sense organic vapours with incorporation of multiwalled carbon nanotubes (MWCNTs) [11]. Polycarbonate blended polysulfone material is recently observed to have improved thermal and mechanical properties[12].

Therefore, investigation of blending compatibility of polycarbonate with other polymer is the urgent need of current research to develop advanced functional materials. All the above mentioned examples relied on laboratory experiments. Usually, preparation of homogeneous blend in wet-lab condition, requires huge time and wastage of materials which can be minimized by in-silico approach through material studio [13] of "Biovia" software.. In present context, we are focusing to optimize the homogeneous blend composition of polybiphrnyldimethylcarbonate (PC) with polyether sulfone (PES) in terms of gas permeability. Among various engineering polymers, polyether sulfone (PES) is a high-temperature sustaining thermoplastic polymer with striking strength and chemical stability from various organic solvents. It belongs to the polysulfone family and contains an aryl-SO_2 subunit in their long chain structures. Nonetheless, the inherent hydrophobic property of PES makes this material sensitive to membrane fouling, restricting its more extensive applications in membrane based water treatment. Due to high chemical stability it is also preferably used for gas separation in harsh environment.

To improve the gas separation efficiency of PES, a few investigations have been performed. In a report, Adib et al. [14] incorporated the nanostructural silica to improve the gas separation. However, blending of PES with other hydrophilic polymer is one of the easiest routes to improve the efficiency of the gas separation. In another report, Mannan et al. [15] investigated the gas-permeation behavior of glassy poly(vinyl acetate) (PVAc)–PES hybrid films and PSF–PES film. Interestingly, it is found that the gas permeation properties of hybrid PSF–PES film is remain unaltered as compared to the properties of polyether sulfone. However on account of the PES–PVAc hybrid polymer, low selectivity was observed for gas separation and may be accounted as the phase separation in their blend. Kamal et al. [16] revealed that the blend with elastomers (like polydimethylsiloxane) leads to the improved gas permeation properties of the polydimethylsiloxane–PES hybrid. Akbarian et al.[17] prepared the PES based blend membranes for CO_2 gas separation with inclusion polyethylene glycol (PEG) as second polymer. Therefore, the present in-silico approach of blend analysis between poly(biphenyl dimethyl carbonate) (PC) and polyether sulfone (PES) may be utilized to optimize the composition to fabricate desirable functional materials with some improved physical and chemical properties.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systems of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polybiphenyldimethylcarbonate (PC) and polyether sulfone were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polybiphenyldimethylcarbonate (PC) on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polybiphenyldimethylcarbonate (PC) and polyether sulfoneas potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Bulk Modulus: Bulk modulus is the measure of the relative change in volume with anunit compressive or tensile stress acting uniformly over its surface. Figure 1 shows that the bulk modulus of the composite decreases linearly with increase in mass fraction of biphenyl dimethyl carbonate.

Shear Modulus: It is defined as the ratio of shear stress and shear strain. It shows the response of the composite to shear deformation. Figure 2 shows that the shearmoduli of the composite decreases linearly with increase in mass fraction of biphenyl dimethyl carbonate.

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Brittle Fracture Stress: Brittle Fracture is the sudden, rapid cracking of a material under stress where the material exhibited practically no evidence of ductility or plastic degradation before the fracture occurs. Figure 5 shows that the brittle fracture stress of the composite decreases linearly with increase in mass fraction of biphenyl dimethyl carbonate.

CONCLUSION

The possibility of use of poly (biphenyl dimethylcarbonate) (PC) and polyether sulfone to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to mechanical properties.The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties decreased with increase in mass fraction of biphenyl dimethyl carbonate. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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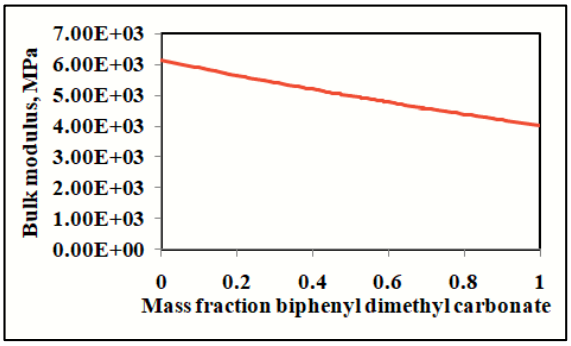

Figure 1. Change in bulk modulus with mass fraction of biphenyl dimethyl carbonate.

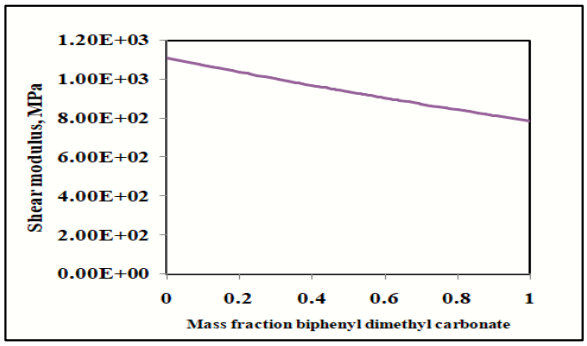

Figure 2. Change in shear modulus with mass fraction of biphenyl dimethyl carbonate.

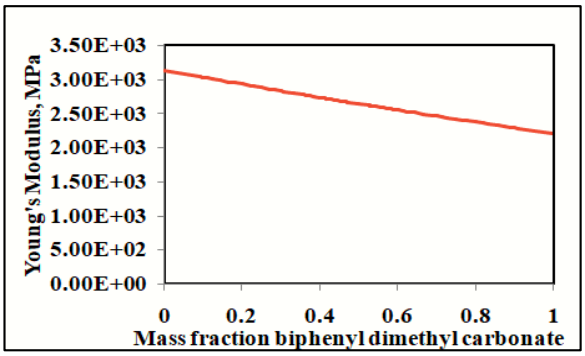

Figure 3. Change in Young's modulus with mass fraction of biphenyl dimethyl carbonate.

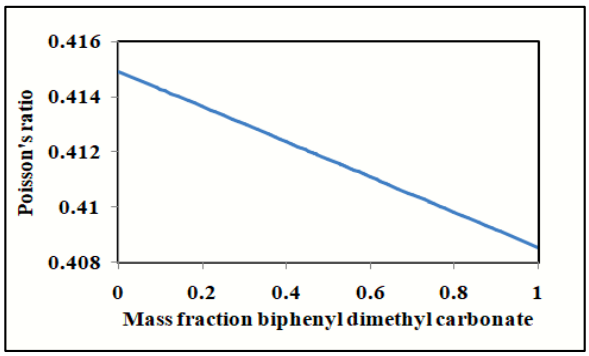

Figure 4. Change in Poisson modulus with mass fraction of biphenyl dimethyl carbonate.

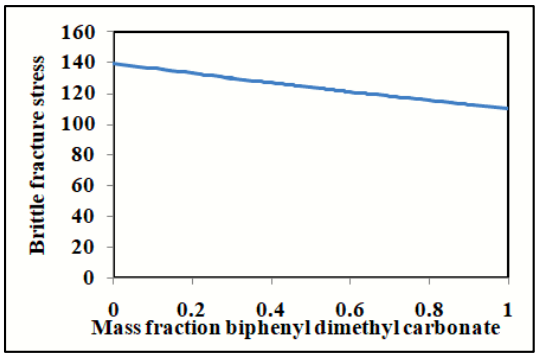

Figure 5. Change in brittle fracture stress with mass fraction of biphenyl dimethyl carbonate.

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyvinyl Alcohol and Polybenzamide Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of polyvinyl alcohol and Polybenzamide to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of vinyl alcohol.This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Mechanical Properties, Silico, polyvinyl alcohol, polybenzamide.

INTRODUCTION

Blends or composites are formed with combination of more than one component where components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisable to combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi-functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance

flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method and this technique is a low cost and less time consuming method. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs.

Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11].The strategy used here for synthesis of poly (benzamide)s relies on polymer end groups being more reactive than the monomer itself resulting in a kinetically controlled living chain-growth polymerization. Because of good control over the polydispersity and the molecular weight, a number of different polymer [12].I Specially synthesized rigid polybenzamide Nano whiskers of approximately 2000 nm length and 200 nm diameter were reported to increase tensile strength and Young's modulus without sacrificing high strainto-failure. [13]. This study is intended to identify the interaction of polyvinyl alcohol and Polybenzamide to form different composite.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and Polybenzamide were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight production of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and Polybenzamide as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of

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Bulk Modulus: Bulk modulus is the measure of the decrease in volume with an increase in pressure. Figure 1 shows that the bulk modulus of the composite increases linearly with increase in mass fraction of vinyl alcohol.

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CONCLUSION

The possibility of use of polyvinyl alcohol and Polybenzamide to form a homogeneous blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to mechanical properties.The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of vinyl alcohol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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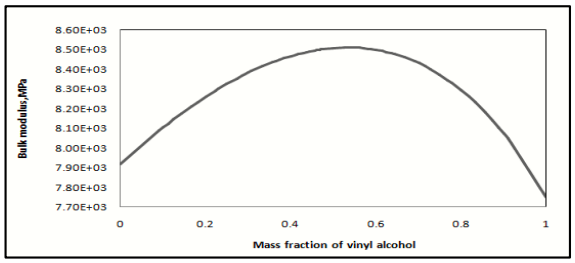

Figure 1. Change in bulk modulus with mass fraction of vinyl alcohol.

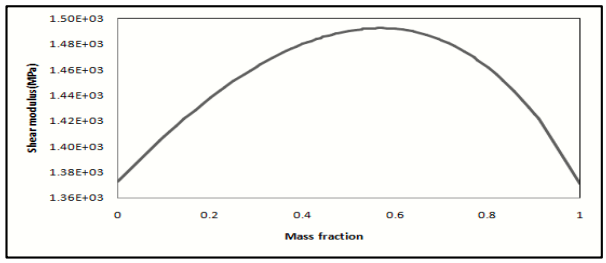

Figure 2. Change in shear modulus with mass fraction of vinyl alcohol.

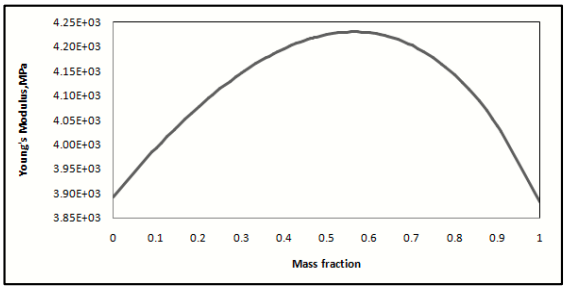

Figure 3. Change in Young's modulus with mass fraction of vinyl alcohol.

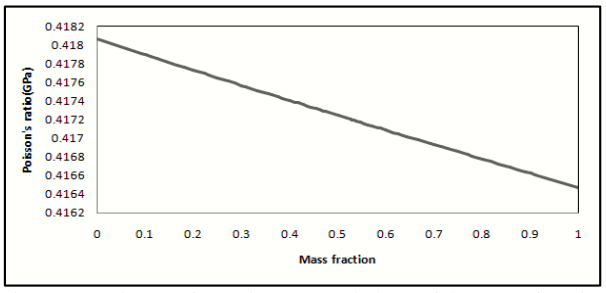

Figure 4. Change in Poisson modulus with mass fraction of vinyl alcohol.

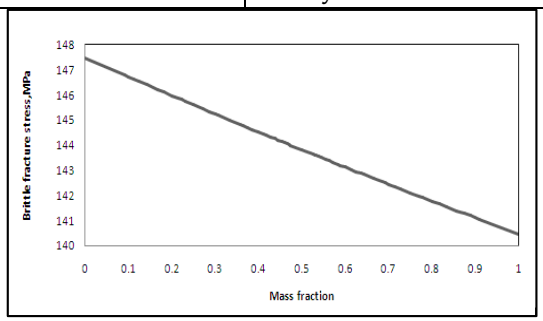

Figure 5. Change in brittle fracture stress with mass fraction of vinyl alcohol.

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyvinyl Alcohol and Poly-1,2-β-D Galactose Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of polyvinyl alcohol and 12bD galact to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of vinyl alcohol.This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: in silico, polyvinyl alcohol, poly-1,2-β-D galactose.

INTRODUCTION

Blends or composites are formed with combination of more than one component where components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisable to combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of

lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method and this technique is a low cost and less time consuming method. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs.

Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11]. Researchers have found applications of glycopolymers (synthetic polymers containing pendant carbohydrate groups) in the separation and removal of toxins and bacteria, tumor cell recognition and glucose-responsive insulin delivery [12]. It has been found that biopolymer blends possess good thermal stability [13].This study is intended to identify the interaction of polyvinyl alcohol and poly-1,2-β-D galactoseto form blend

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and poly-1,2-β-D galactosewere fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly-1,2-β-D galactoseas potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

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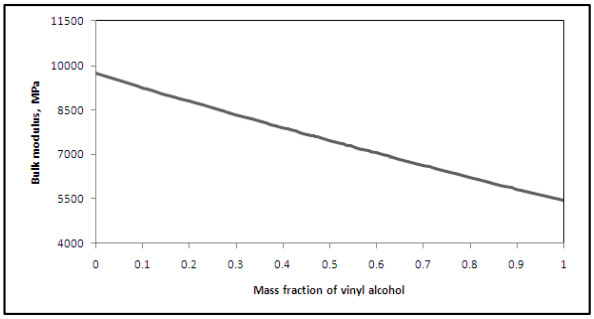

Figure 1. Change in bulk modulus with mass fraction of vinyl alcohol.

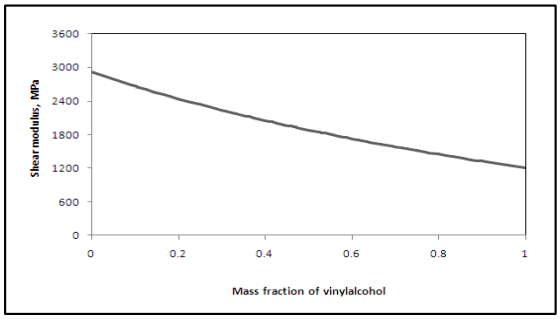

Figure 2. Change in shear modulus with mass fraction of vinyl alcohol.

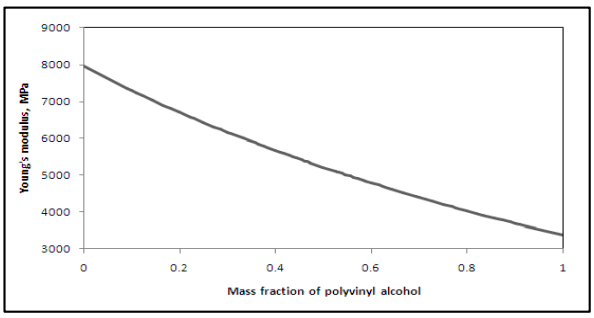

Figure 3. Change in Young's modulus with mass fraction of vinyl alcohol.

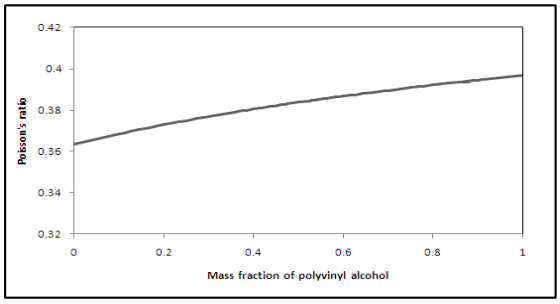

Figure 4. Change in Poisson modulus with mass fraction of vinyl alcohol.

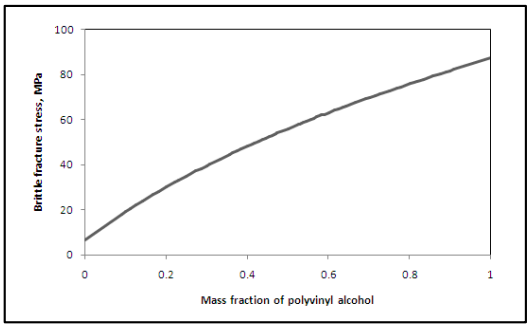

Figure 5. Change in brittle fracture stress with mass fraction of vinyl alcohol.

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RESEARCH ARTICLE

In silico Analysis of Mechanical Properties of Polyvinyl Alcohol and Poly-1,3-α-D-Galactose

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of polyvinyl alcohol and Poly-1, 3-α-D-Galactose to provide desired mechanical properties of the blend was explored using Biovia Materials Studio. The mechanical properties of the composite were studied based on bulk modulus, shear modulus, Young' modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of vinyl alcohol.This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Silico, polyvinyl alcohol, Poly-1, 3-α-D-Galactose

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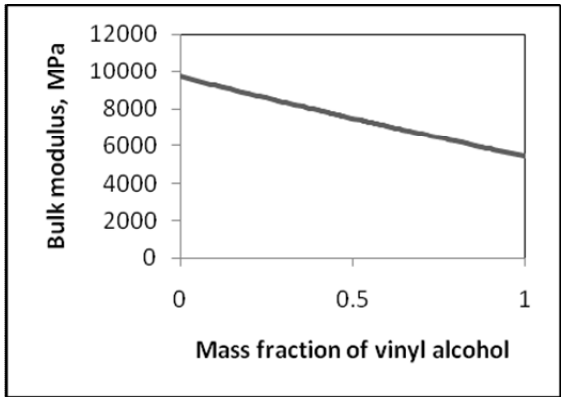

Figure 1. Change in bulk modulus with mass fraction of vinyl alcohol.

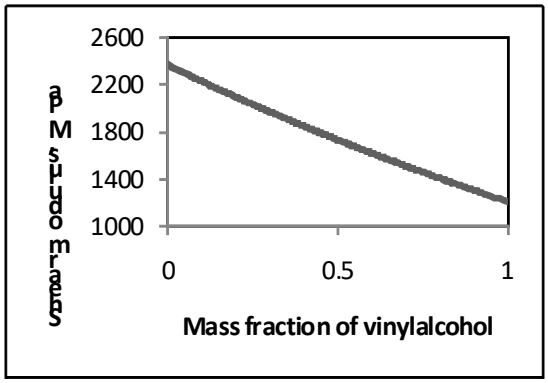

Figure 2. Change in shear modulus with mass fraction of vinyl alcohol.

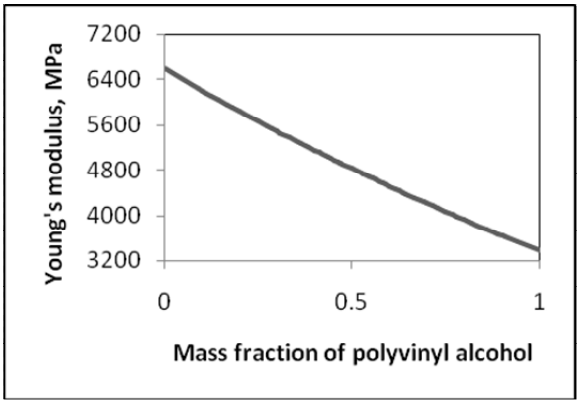

Figure 3. Change in Young's modulus with mass fraction of vinyl alcohol.

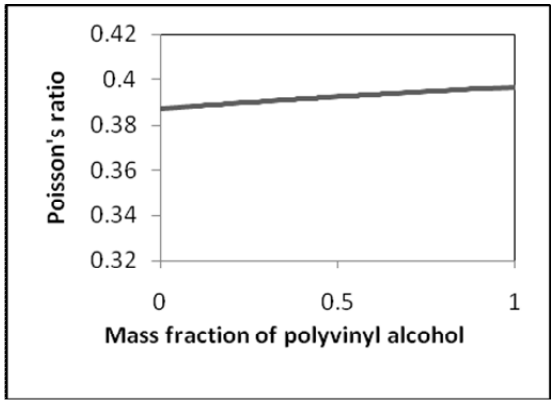

Figure 4. Change in Poisson modulus with mass fraction of vinyl alcohol.

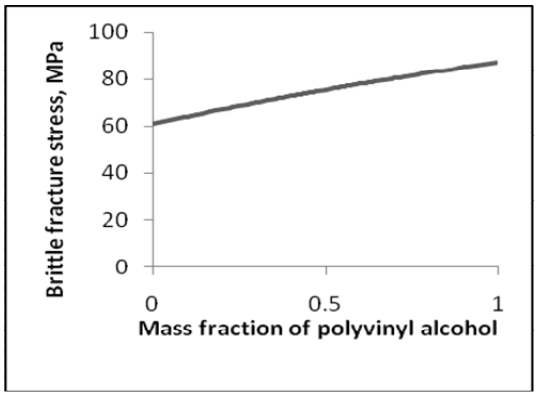

Figure 5. Change in brittle fracture stress with mass fraction of vinyl alcohol.

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Poly Acrylic Acid and Polyoxyethylene Composite

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ABSTRACT

A blend is a combination of more than one components. The desired property of a blend is its homogeneity. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all those parameters increased with increase in mass fraction of polyvinyl alcohol. This study will help verify pairs without performing laboratory experiments saving equipment, currency and time.

Keywords: Synthia; Insilico; Polyacrylic acid; Polyoxyethylene, thermal and dielectric properties

INTRODUCTION

Blends or composite are resources containing more than one part. The components do retain their identity in the combination. As it is very difficult to find multiple properties in a single material, it is advisable to combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the preferred property. Thus a blend saves time to develop a new material thereby dipping the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn significant attention in recent years. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high

strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) has been used to identify compatible pairs. Acrylic acid have a board varity of application in dentistry as denture bases, artificial teeth , denture repair material, maxillofacial appliances for skeletal defects etc.[8] , bone repair [9] dispersing agent, superabsorbent polymer ion replace resin,etc. [10] Polyacrylic acid is a polyelectrolyte soluble in aqueous media at impartial pH It is used for prepare hydrogels. It is not poisonous and does not reason irritation [11]. The area of high pressure molecular credence polymers deliberate were poly (oxythylene) homopolymers (polyox) with molecular with molecular credence ranging from 4,000,000 to 7,000,000 power characteristics optional fine flow ability for these resources and predicted case fulfil importance uniformity irritation[12].

Experiments showed a precise extreme notch of bulge for these resources in equality gastric and shock absorber solution[13]. These polymers bottle sustain the discharge percentage of mutually water-soluble and indecipherable drugs from drug providing system. The soothing molecular burden polymers control a fewer marked sustained-release provoke compare to the eminent molecular authority polymer data (i.e individual with 7,000,000 molecular weight).Intensification in the freedom percentage of the drug. The solubility of the drugs openly influenced the make available rate. Discharge kinetics were evaluated and appeared to be influenced by the molecular import of the polymer, the solubility of medicine, and the ratio of the drug to the polymer in the capsule [14]. Biomodal issue kinetics was exhibit by a amount of furosemide formulation (i.e. F5and F8).

MATERIALS AND METHODS

Software Used: Equipment studio module of Biovia software (Dassaults system of France) was old for study. The software utilize piece of equipment education techniques and usual algorithms to calculate the degree of communication.

Methodology: Polyacrylic acid and oxyethelene were prepared by the synthia menu resources studio. It was subsequently enclose for characteristic weight fraction of the components. Varied properties of the composite were displayed in a tabular form. The ethics were second-hand to plot graphs to make out the impression of result little bit of poly-acryalic acid on the themal properties of the composite.

RESULTS AND DISCUSSION

In this work the use of poly acrylic acid and poly oxyethylenes as potential components of a composite was analyzed using Biovia equipment Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to calculate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group involvement cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of

group contributions is required and properties may be predicted for any polymer composed of any mixture of the subsequent the thermal properties of the composite were premeditated based on Cp of the solid, thermal conductivity, dielectric constant.

Heat Capacity: Heat capacity is defined as the amount of heat to be supplied to a given mass of a material to produce a unit change in its temperature**.** Figure 1 shows that increase in heat capacity of the composite with increase in mass fraction of acrylic acid.

Thermal Conductivity: Thermal conductivity refers to the intrinsic ability of a material to transfer or conduct heat. Figure 2 shows that the thermal conductivity of the composite decrease with increase in mass fraction of poly acrylic acid.

Dielectric Constant: The dielectric constant is the ratio of the permittivity of a substance to the permittivity of free space .it is dimensionless value and is also called relative permittivity. Figure 3 shows that the dielectric constant of the composite increase with increase in mass fraction of acrylic acid.

CONCLUSION

The opportunity of exhaust of Polyacrylic acid and oxyethelene to type bring together was explored by Biovia Material Studio. The arrangement of the merger was analyzed with regard to heat capacity, thermal conductivity, dielectric constant. The results indicated that all the three parameters and one parameter is decrease in increase with increase in mass fraction of poly acrylic acid other two parameter increase with increase in mass fraction of acrylic acid. As a rule apparatus for a m? are identified experimentally. This in sillico examine will stop find out working of a merge without performing arts laboratory experiments materials, funds and time.

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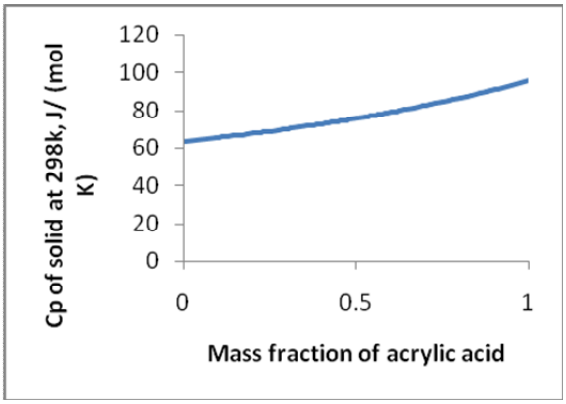

Figure 1. Change in heat capacity with mass fraction of acryalic acid

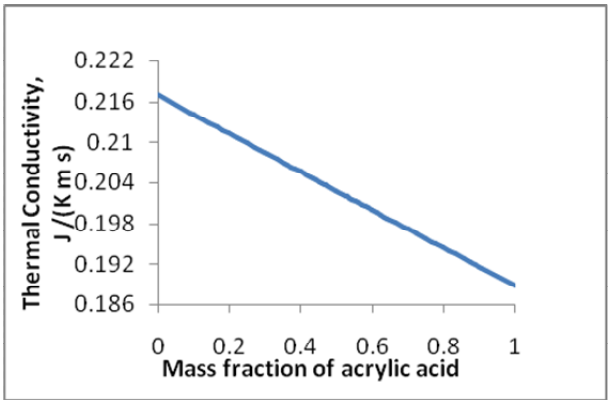

Figure 2. Change in thermal conductivity with mass fraction of acrylic acid

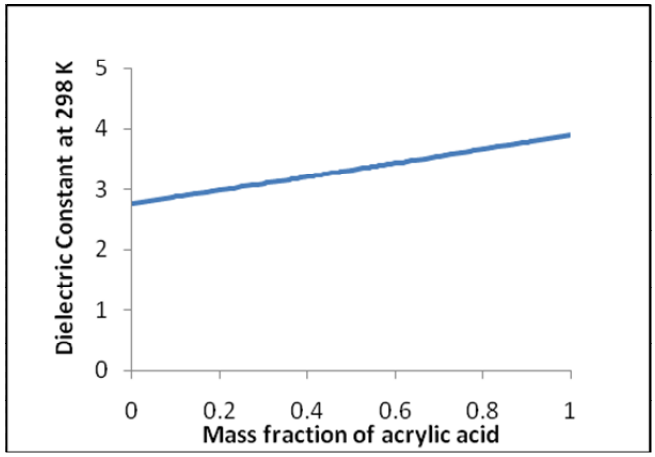

Figure 3. Change in dielectric constant with mass fraction of acrylic acid

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RESEARCH ARTICLE

In silico Analysis of Gas Permeability Properties of Poly Acrylic Acid and Polyoxyethylene Composite

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ABSTRACT

A blend is a combination of more than one components. The desired property of a blend is its homogeneity. The composition poly acrylic acid and poly oxythylene to provide desired mechanical property of the blend was explore using Biovia Materials Studio. The composition of the blend was analyzed with respect to permeability property. The molar volume and density decreased with increase in poly acrylic acid fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases decrease with increase in mass fraction of polyvinyl alcohol. This learning will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Synthia; Insilico; Polyacrylic acid; Polyoxyethylene,gas permeability

INTRODUCTION

Blends or composite are resources containing more than one part. The components do retain their identity in the combination. As it is very difficult to find multiple properties in a single material, it is advisable to combine different components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the preferred property. Thus a blend saves time to develop a new material thereby dipping the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn significant attention in recent years. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance.

Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers; latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments.

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Experiments showed a precise extreme notch of bulge for these resources in equality gastric and shock absorber solution[13]. These polymers bottle sustain the discharge percentage of mutually water-soluble and indecipherable drugs from drug providing system. The soothing molecular burden polymers control a fewer marked sustained-release provoke compare to the eminent molecular authority polymer data (i.e individual with 7,000,000 molecular weight). Intensification in the freedom percentage of the drug. The solubility of the drugs openly influenced the make available rate. Discharge kinetics were evaluated and appeared to be influenced by the molecular import of the polymer, the solubility of medicine, and the ratio of the drug to the polymer in the capsule[14]. Biomodal issue kinetics was exhibit by a amount of furosemide formulation (i.e. F5and F8).

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RESULTS AND DISCUSSION

In this work the use of poly acrylic acid and poly oxyethylenes as potential components of a composite was analyzed using Biovia equipment Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to calculate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer

contains a group for which the group involvement cannot be estimated, then the property of that polymer cannot be calculated. To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any mixture of the subsequent nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Molar Volume: The molar volume occupied by one mole of a substance at given at a given temperature and pressure. Figure 1 shows that the molar size of the composite decrease linearly with rise in dimension small part of mass fraction of acrylic acid.

Density: The density in increase indicates drop in porosity. An advance porosity will enhance the float up part creation in apposite for absorption application. Figure 2 shows that the density of the composite increase linearly with growth in bulk part of acrylic acid.

Permeability of Gas: Permeability is the rate by which the gas can pass through the polymer membrane following the gas has come to equilibrium. Lower permeability indicate longer time lag for the gas to pass through the membrane. Figure 3 shows that the permeability of oxygen through the composite decreases with increase in mass division of acrylic acid.

Figure 4 shows that the permeability of nitrogen through the composite decrease with increase in mass fraction of acryalic acid. Figure-5 shows that the permeability of carbon dioxide through composite decrease with increases of mass fraction poly acrylic acid. As a consequence the domino effect indicated that an multiply in polyacryalic acid little bit reduces the permeability capacity be weight by the molecular import of the gases.

CONCLUSION

Possibility of use poly acrylic acid and poly oxyethylene to form a homogeneous blend was explore using Biovia equipment Studio. The composition of the blend was analyzed with respect to permeability properties. The molar volume and density decreased with increase in poly acrylic acid. The permeability property of the composite was studied based on permeability of oxygen, nitrogen and carbon dioxide. The results indicated that the permeabilityfor all the gases decreased with increase in mass fraction of vinyl alcohol. Usually components for a blend are recognized experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving equipment, currency and time.

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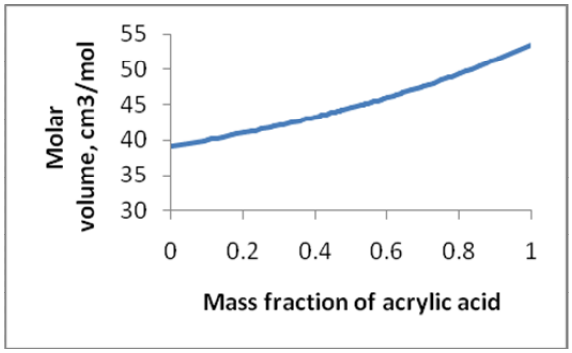

Figure 1. Change in molar volume with mass fraction of acrylic acid

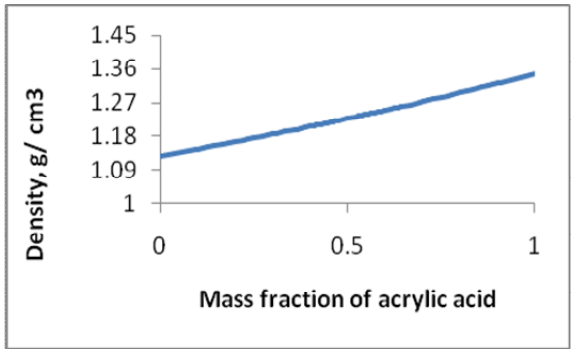

Figure 2. Change in density with mass fraction of acrylic acid

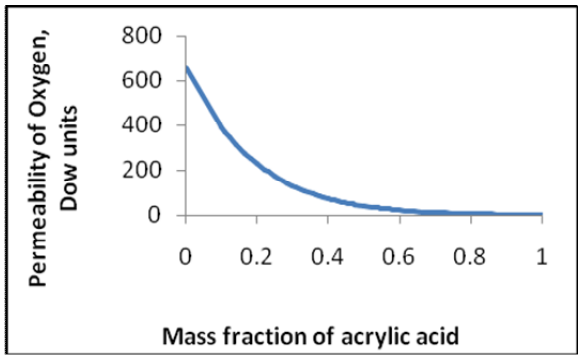

Figure 3. Change in permeability of oxygen with mass fraction of acrylic acid

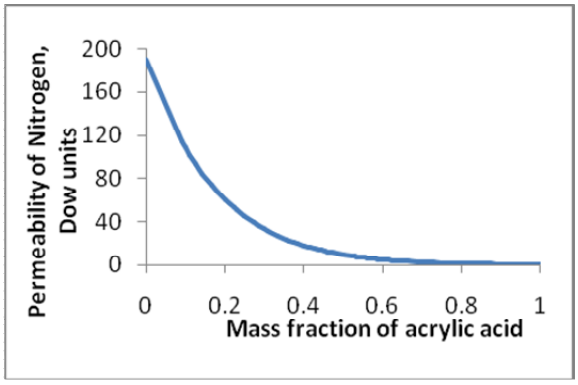

Figure 4. Change in permeability of nitrogen with mass fraction of acrylic acid

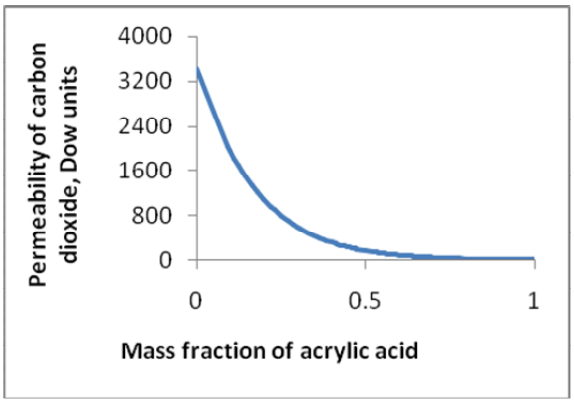

Figure 5. Change in permeability of carbon dioxide with mass fraction of acrylic acid

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyvinyl Alcohol and Polyethylene Terephthalate Composite

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Received: 16 Mar 2020 Revised: 18 Apr 2020 Accepted: 22 May 2020

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ABSTRACT

A blend is a combination of more than one component. The desired property of a blend is its homogeneity. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all those parameters increased with increase in mass fraction of polyvinyl alcohol. This study will help verify pairs without performing laboratory experiments saving equipment, currency and time.

Keywords: Synthia, In Silico, Poly Ethylene Terephthalate, Thermal and Dielectric properties

INTRODUCTION

Blends or composites to be formed with combination of more than one component where components do retain their identity in the mixture. As it is very difficult to find multiple properties in a single material, it is advisable to mix dissimilar components thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of improvement of products with desired properties. Polymer blends can be made of two or more polymers, or fibers and polymer, or particles and polymer.

Nano material customized polymers paved the way to multi useful materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire evidence materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy lacking increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite material having high strength important for enhancing fuel efficiency in the field of transport [5]. There is application of composites in structural Engineering due to high strength to weight ratio

and resistance to decay. Thus, glass fiber durable polymers; latex polymer cementitious composites [6] were developed for building of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mention example relied on laboratory experiments. Usually blends are prepared by test and fault method andthis method is a low cost and less time consuming method. Thus, researchers have focused on the use of in silico move toward to develop new blends. Software (Materials Studio [7]) has been used to identify well-matched pairs. Among the a mixture of polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, simple film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is extensively used in covering industry to form strong polymeric films. It is because of their high mechanical power, environmental stability and easy processability [10]. On the other hand, PVA is poisonous, semicrystalline, hydrophilic, biocompatible and simply soluble in water [11].

The consumption of plastics in Western Europe is of 38 million tonnes per year, the majority of which are used in the production of plastic packaging, household and domestic products, electrical and electronic goods [12]. There is also significant consumption of plastics for the structure and construction industry and automotive industry. The two main types of plastics are thermoplastics, which soften when heated and harden again when cooled, and thermosets, which harden by curing and cannot be re-moulded. About 80 % of plastics used in Western Europe are thermoplastics [13].For many waste landfills is the largest route for disposal throughout the countries of Europe. For some countries, including Lithuania, more than 60 % of municipal solid waste is disposed of to landfill [14]. Plastics make up high proportion of waste that volume and range used increases dramatically. Although plastics make up between 5 wt.% and 15 wt.% of municipal solid waste it comprises 20 % – 30 % of the volume [13]. Most plastics are non-degradable and take a long time to decompose, possibly up to hundreds of years – although no-one knows for certain as plastics have not existed for long enough, when they are landfilled.

It is estimated that only about 50 % of the plastics produced in Western Europe each year are available for collection and recycling [12 – 14]. According to the experts from Kaunas University of Technology in Lithuania plastics reach about 82 thousands tones of municipal solid waste in 2004. It comprised about 24 kg for one inhabitant [15]. Waste recycling in Lithuania increases constantly andduring 2000–2006 it ranges between 20 – 35 thousand tonnes per year [16]. According to the Environmental Protection Agency (EPA) "recycling" is considered to be processing of waste to make new article. There are divided three distinct approaches to the recycling of post-consumer plastic materials: 1) it could be reused directly; 2) undergo physical reprocessing, for example, grinding, melting and reforming; 3) be subjected to chemical treatment, when components are isolated and reprocessed for use in manufacture. A new widespread nomenclature of recycling was adopted by EPA. Primary recycling involves the use of pre-consumer industrial scrap and salvage, while physical reprocessing refers as secondary recycling and chemical processing as tertiary recycle [16].

MATERIALS AND METHODS

Software Used: Equipment studio part of Biovia software (Dassault Systemes of France) was used for analysis. The software utilize machine study techniques and normal algorithms to predict the level of interaction.

Methodology: The structure of polyvinyl alcohol andpoly ethylene Terephthalatewere fed to the synthia menu of equipment Studio. It was then run for different weight fractions of the mechanism. Different property of the composite was displayed in a tabular form. The values to be used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the thermal and dielectric properties of the composite.

RESULTS AND DISCUSSION

The use of polyvinyl alcohol andpoly ethylene Terephthalate as potential mechanism of a composite was analyze using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-define correlation (advanced quantitative structure-property relationships) to estimate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Accordingly, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic relations that give rise to it. However, the main shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculate.To overcome this limitation, the technique implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from diagram theory are employed. The thermal properties of the composite were premeditated based on Cp of the solid, thermal conductivity, dielectric constant.

Heat Capacity: Heat capacity is defined as the amount of heat to be supplied to a given mass of a material to produce a unit change in its temperature Figure 1 shows that decrease in heat capacity of the composite with increase in mass fraction of vinyl alcohol.

Thermal Conductivity: Thermal conductivity refers to the intrinsic ability of a material to transfer or conduct heat. Figure 2 shows that the thermal conductivity of the composite decrease with increase in mass fraction of vinyl alcohol.

Dielectric Constant: The dielectric constant is the ratio of the permittivity of a substance to the permittivity of free space .it is dimensionless value and is also called relative permittivity. Figure 3 shows that the dielectric constant of the composite increase with increase in mass fraction of vinyl alcohol.

CONCLUSION

The opportunity of exhaust poly vinyl alcohol polyethylene terephthalate to type a bring together was explored by Biovia resources studio. The arrangement of the merger was analyzed with regard to heat capacity, thermal conductivity, dielectric constant. The results indicated that all the three parameters and one parameter is decrease in increase with increase in mass fraction of poly acrylic acid other two parameter increase with increase in mass fraction of acrylic acid. As a rule apparatus for a m? are identified experimentally. This in sillico examine will stop find out working of a merge without performing arts laboratory experiments materials, funds and time.

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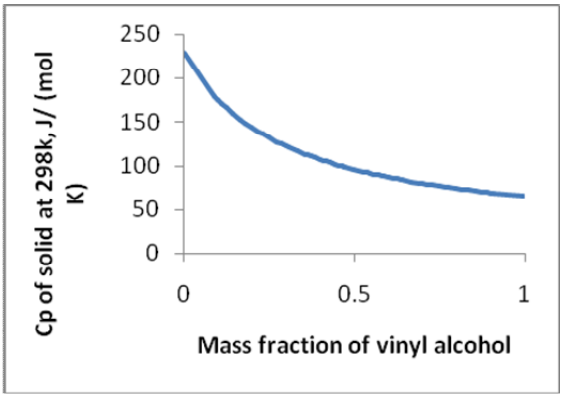

Figure 1. Change in heat capacity with mass fraction of vinyl alcohol

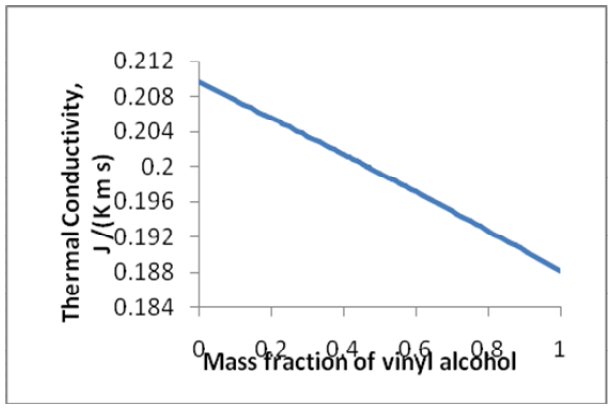

Figure 2. Change in thermal conductivity with mass fraction of vinyl alcohol

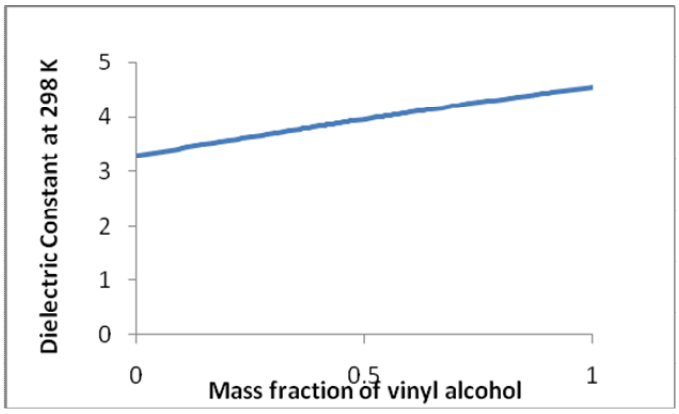

Figure 3. Change in dielectric constant with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Poly (Biphenyl Dimethyl Carbonate) and Polydimethylsiloxane Composite

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ABSTRACT

Polymeric blend is a reasonable suggested method to obtain the new polymer materials having properties better to those of the individual constituents. Dielectric constant is an important parameter to judge a better dielectric material. Further, polymer blend with high thermal properties can be used in various packaging industry. In this paper, the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. From the results it was noticed that all those parameters increased with increase in mass fraction of poly biphenyldimethyl carbonate. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Blend; Biovia Material Studio; Dielectric constant; Thermal properties; Polybiphenyldimethyl carbonate; *In silico* analysis

INTRODUCTION

Recently, Researchers have given more attention towards fabrication of good dielectric materials and high thermal stable materials because of their many applications in industry. For better dielectric material it is very much important to find out the various important parameters such as such as high dielectric constant, low dielectric loss [1]. Further, thermal properties of the material are used to judge the high thermal stable material. Therefore polymer is becoming hot field of science and technology to act as a good dielectric and thermal stable material. But there are certain limitations for synthesis of new polymer such as synthesis technology, cost of production and source of raw material. Hence, blending polymers is a reasonable proposed technique to achieve the new polymer materials, having properties of the designed material better to those of the individual constituents. Polymer blends are generally simpler process and have fantastic flexibility. These have many applications in the field of electronic industry. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4].

Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementations composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.

In present context, the dielectric and thermal properties of blend are analyzed containing polybiphrnyl dimethylcarbonate (PC) with polydimethylsiloxane (PDMS). It is a polymeric organosilicon compound, particularly known for its unusual rheological behaviors. Moreover it is optically clear, non-toxic and non-flammable. Polydimethyl siloxane (PDMS) shows wide applications like contact lenses, medical devices and preparing elastomer materials. It is also used in making of lubricants and heat-resistant tiles. Recently, the PDMS based blend membranes with polyvinyl chloride-co-vinyl acetate (PVCA)were synthesized for CO_2 seperation [17]. Polydimethyl siloxane is also used in biomedical application like maxillofacial prosthetics, artificial blood vessels and articular cartilage replacement, when it is blended with poly ether (ether) ketone (PEEK) [18]. The present in-silico approach of blend analysis between poly biphenyldimethyl carbonate (PC) and polydimethyl siloxane (PDMS) may be utilized to know the good dielectric and thermal properties at optimized ratio.Therefore, the dielectric constant and thermal properties of the blend is studied with different acrylic acid proportions.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polybiphenyldimethyl carbonate and Polydimethyl siloxane were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of poly biphenyldimethyl carbonate on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polybiphenyldimethyl carbonateand Polydimethyl siloxaneas potential components of a composite was analyzed using Biovia Materials Studio. Biovia Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Heat Capacity: It is the amount of heat required to raise the temperature of one unit weight of a substance by 1°C without change of phase. Figure 1 shows that the heat capacity (Cp) of the composite decreases linearly with increase in mass fraction of poly biphenyldimethyl carbonate.

Thermal Conductivity: It indicates the correlation between heat flux per unit area and temperature gradient. It refers to the intrinsic ability of a material to transfer heat. Figure 2 shows that the thermal conductivity of the composite increases linearly with increase in mass fraction of biphenyldimethyl carbonate.

Dielectric Constant: It is defined as the ratio of the electric permeability of the material to the electric permeability of free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant. Figure 3 shows that the dielectric constant of the composite increases with increase in mass fraction of biphenyldimethyl carbonates.

CONCLUSION

Different properties the blend of polybiphenyldimethyl carbonate and Polydimethyl siloxane was analyzed using Biovia Materials Studio. Because of enhance of different properties such as dielectric constant and thermal it can be used in various applications. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all the three parametersincreased with increase in mass fraction of acrylic acid so that his blend with high biphenyldimethyl carbonate proportions can be used in various applications Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments with low cost.

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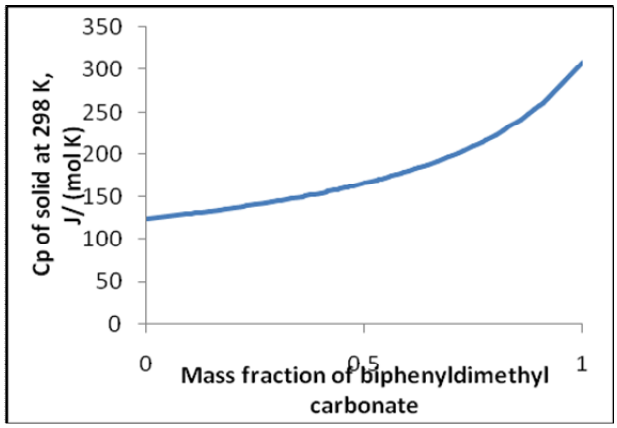

Figure 1. Change in heat capacity with mass fraction of biphenyldimethyl carbonate

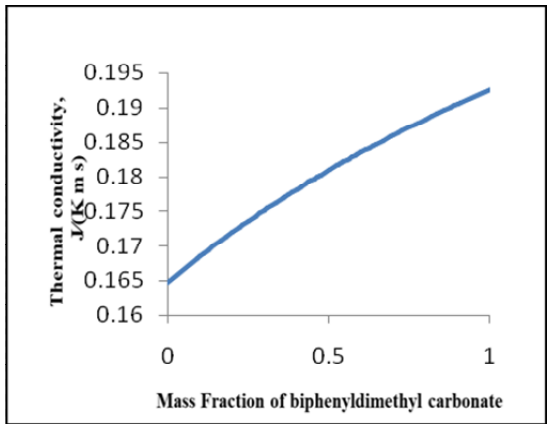

Figure 2. Change in thermal conductivity with mass fraction of biphenyldimethyl carbonate.

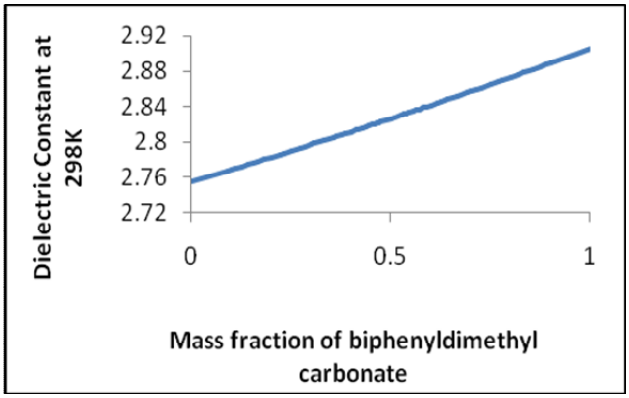

Figure 3. Change in dielectric constant with mass fraction of biphenyldimethyl carbonate

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyacrylic Acid and Poly (1, 2-α-D-Galactose) Composite

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ABSTRACT

Blending polymers is a reasonable proposed technique to achieve the new polymer materials having properties better to those of the individual constituents. Dielectric constant is an important parameter to judge a better dielectric material. Further, polymer blend with high thermal properties can be used in various packaging industry. In this paper, the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. From the results it was noticed that all those parameters decreased with increase in mass fraction of acrylic acid so that the value of these parameters will increase with increase in mass fraction of α-D-galactose. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Blend; Biovia Material Studio; Dielectric constant; Thermal properties; Polyacrylic acid; In silico analysis

INTRODUCTION

Dielectric materials have drawn considerable attention because of their many applications in industry. For better dielectric material it is very much important to find out the various important parameters such as such as high dielectric constant, low dielectric loss [1]. Further, thermal properties of the material are considered for the use of materials in various applications such as packaging industry. Therefore polymer is becoming hot field of science and technology for scientist. But there are certain limitations for synthesis of new polymer such as synthesis technology, cost of production and source of raw material. Hence, blending polymers is a reasonable proposed technique to achieve the new polymer materials, having properties of the designed material better to those of the individual constituents. Polymer mixes are generally simpler process and and have fantastic flexibility. These have many applications in the field of electronic industry. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without

increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.

Acrylic acid is an organic compound which contains a vinyl group attached to carboxylic acid. It can be used in various purpose such as dispersing agent, artificial teeth and bone repair because of its biocompatibility, biodegradability nature and low toxicity [8-10]. Polyacrylic acid as water soluble polymer have been given as special attention because it can be applied in various applications such as ion exchange, efficient corrosion inhibitor and capacitorsand also it is used for preparing hydrogels. It is not toxic and does not cause irritation [11].

Researchers have used D-galactose in combination with other materials to different applications [12]. Poly-1, 2-α-D-galactose has been reported to be used in Curtius reaction.This study is intended to find out the change of gas permeability value of blend of polyacrylic acid and poly-1, 2-α-D-galactose with different proportions. In this paper, the change in thermal and dielectric properties of blend is analyzed with respect to the change in acrylic acid proportions theoretically. From thermal properties, it can be found the thermal stability of the blend. Further, the dielectric constant of the blend is studied with different acrylic acid proportions.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyacrylic acid and poly-1, 2-α-D-galactosewere fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyacrylic acidon the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyacrylic acidand poly-1, 2-α-D-galactoseas potential components of a composite was analyzed using Biovia Materials Studio. Biovia Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of

group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Heat Capacity: It is the amount of heat required to raise the temperature of one unit weight of a substance by 1°C without change of phase. Figure 1 shows that the heat capacity (Cp) of the composite decreases linearly with increase in mass fraction of acrylic acid.

Thermal Conductivity: It indicates the correlation between heat flux per unit area and temperature gradient. It refers to the intrinsic ability of a material to transfer heat. Figure 2 shows that the thermal conductivity of the composite decreases linearly with increase in mass fraction of acrylic acid.

Dielectric Constant: It is defined as the ratio of the electric permeability of the material to the electric permeability of free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant. Figure 3 shows that the dielectric constant of the composite decreases with increase in mass fraction of acrylic acid.

CONCLUSION

Different properties the blend of polyacrylic acidand poly-1, 2-α-D-galactosewas analyzed using Biovia Materials Studio. Because of enhance of different properties such as dielectric constant and thermal it can be used in various applications. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all the three parameters decreased with increase in mass fraction of acrylic acid so that all the three parameters will increase with increase in mass fraction of α-D-galactose. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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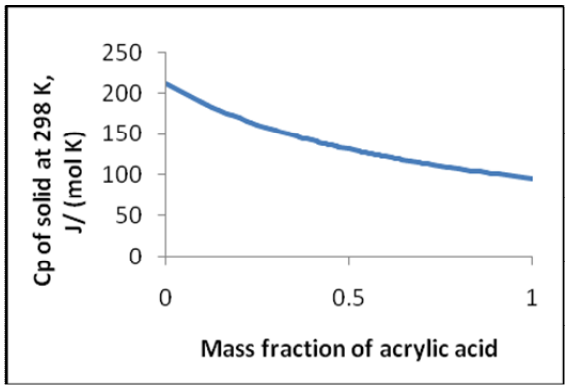

Figure 1. Change in heat capacity with mass fraction of acrylic acid

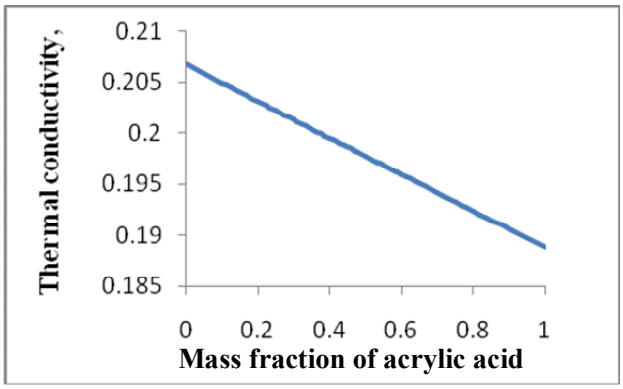

Figure 2. Change in thermal conductivity with mass fraction of acrylic acid

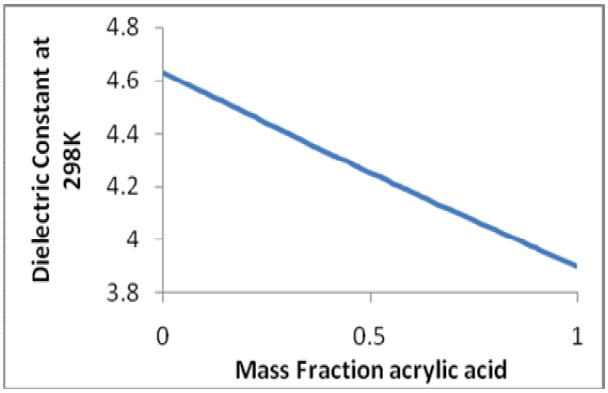

Figure 3. Change in dielectric constant with mass fraction of acrylic acid

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyvinyl Alcohol and Poly (Biphenyl Dimethyl Carbonate) Composite

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ABSTRACT

In this paper, we have tried to explore the thermal and dielectric property of polyvinyl alcohol and poly (biphenyl dimethyl carbonate) to form a miscible blend using Biovia Materials Studio. Usually, blend is a mixture of two or more components and expected to have homogeneity. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all those parameters increased with increase in mass fraction of vinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: In silico, thermal and dielectric properties, polyvinyl alcohol and poly(biphenyl dimethyl carbonate), Synthia, Biovia

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties. Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi-functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of

transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.

Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11].

Poly (biphenyl dimethyl carbonate) has an amorphous structure and is considered to be an engeeniering plastic. Its wide applications include impact resistance, strength, high temperature performance, toughness, load bearing capabilities, dimensional stability, flame retarding capabilities, and excellent optical clarity. Based on these properties they have commercialized as outdoor signs, eye glasses, compact disks, CD-ROM, aircraft windows, automotive windows and instrument panels, food trays and containers, automotive headlamp covers, housings of appliances, and medical devices [12, 13]. It has been found that biopolymer blends possess good thermal stability [14]. This study is intended to explore the thermal and dielectric properties of the blends developed by varying the mass fraction of polyvinyl alcohol and poly (biphenyl dimethyl carbonate) using synthia.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and poly(biphenyl dimethyl carbonate) were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly(biphenyl dimethyl carbonate) as potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Heat Capacity: It is the amount of heat required to raise the temperature of one unit weight of a substance by 1°C without change of phase. Figure 1 shows that the heat capacity (Cp) of the composite decreases with increase in mass fraction of vinyl alcohol.

Thermal Conductivity: It indicates the correlation between heat flux per unit area and temperature gradient. It refers to the intrinsic ability of a material to transfer heat. Figure 2 shows that the thermal conductivity of the composite decreases linearly with increase in mass fraction of vinyl alcohol.

Dielectric Constant: It is defined as the ratio of the electric permeability of the material to the electric permeability of free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant. Figure 3 shows that the dielectric constant of the composite increases linearly with increase in mass fraction of vinyl alcohol.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly(biphenyl dimethyl carbonate) to form a blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that heat capacity and thermal conductivitydecreased with increase in mass fraction of vinyl alcohol whereas the dielectric constant increases. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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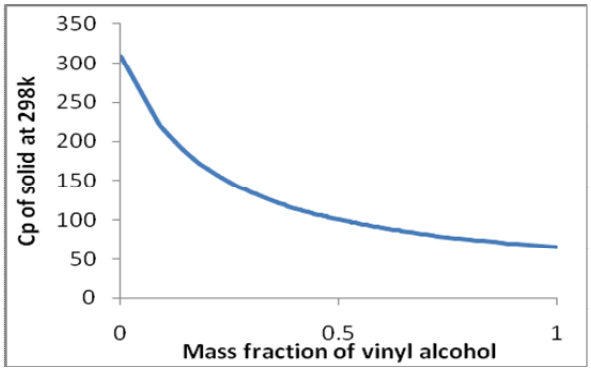

Figure 1. Change in heat capacity with mass fraction of vinyl alcohol

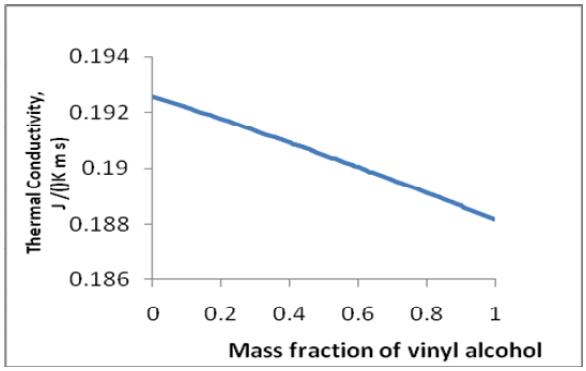

Figure 2. Change in thermal conductivity with mass fraction of vinyl alcohol

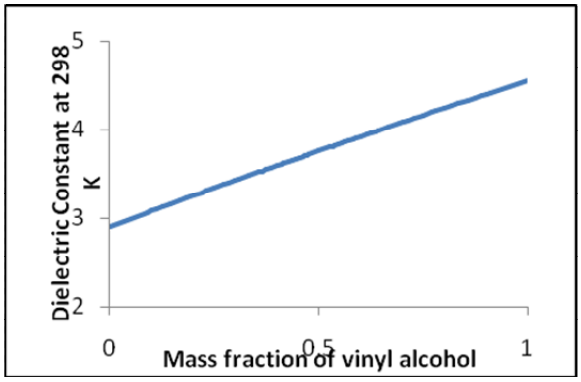

Figure 3. Change in dielectric constant with mass fraction of v inyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyvinyl Alcohol and Polybenzamide Composite

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ABSTRACT

A blend is a mixture of more than one components. The desired property of a blend is its homogeneity. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all those parameters increased with increase in mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Thermal and dielectric properties, Silico, polyvinyl alcohol, polybenzamide

INTRODUCTION

Blends or composites are materials containing more than one components. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials, mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were

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Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11]. The strategy used here for synthesis of poly(benzamide)s relies on polymer end groups being more reactive than the monomer itself resulting in a kinetically controlled living chain-growth polymerization. Because of good control over the polydispersity and the molecular weight, a number of different polymer [12].Polybenzamide have been reported to be used in Curtius reaction. This study is intended to identify the interaction of polyvinyl alcohol and polybenzamide to form composite.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and polybenzamide were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

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To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Heat Capacity: It is the amount of heat required to raise the temperature of one unit weight of a substance by 1°C without change of phase. Figure 1 shows that the heat capacity (Cp) of the composite increases linearly with increase in mass fraction of vinyl alcohol.

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CONCLUSION

The possibility of use of polyvinyl alcohol and polybenzamideto form a blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all the three parametersincreased with increase in mass fraction of vinyl alcohol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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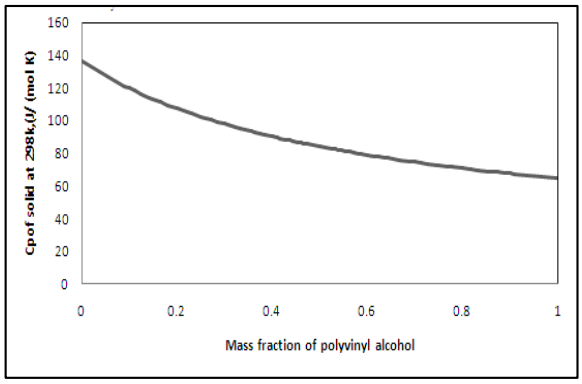

Figure 1. Change in heat capacity with mass fraction of vinyl alcohol

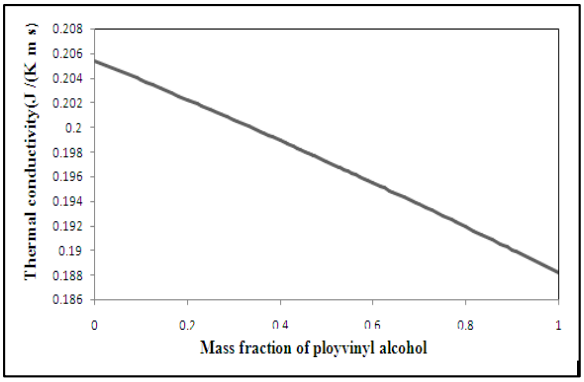

Figure 2. Change in thermal conductivity with mass fraction of vinyl alcohol

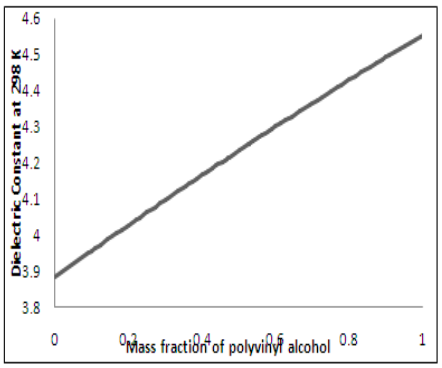

Figure 3. Change in dielectric constant with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyvinyl Alcohol and Poly-1,2-β-D Galactose Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all those parameters increased with increase in mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Thermal and dielectric property, in silico, polyvinyl alcohol, poly-1,2-β-D galactose.

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials[3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancy without increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were

developed for construction of bridges, light rail transit, mining and tunneling, retaining walls and other waterside buildings. All the above mentioned examples relied on laboratory experiments. Usually blends are prepared by trial and error method. Thus it involves wastage of materials, time and money. Thus, researchers have focused on the use of in silico approach to develop new blends. Software (Materials Studio [7]) have been used to identify compatible pairs.

Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11]. Researchers have found applications of glycopolymers (synthetic polymers containing pendant carbohydrate groups) in the separation and removal of toxins and bacteria, tumor cell recognition and glucose-responsive insulin delivery [12]. It has been found that biopolymer blends possess good thermal stability [13].This study is intended to identify the interaction of polyvinyl alcohol and poly-1,2-β-D galactoseto form blend.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and poly-1,2-β-D galactose were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly-1,2-β-D galactoseas potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Heat Capacity: It is the amount of heatrequired to raise the temperature of one unit weight of a substance by 1°C without change of phase.Figure 1 shows that the heat capacity (Cp) of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Thermal Conductivity: It indicates the correlation between heat flux per unit area and temperature gradient.It refers to the intrinsic ability of a material to transfer heat.Figure 2 shows that the thermal conductivity of the composite increases linearly with increase in mass fraction of vinyl alcohol.

Dielectric Constant: It is defined as the ratio of the electric permeability of the material to the electric permeability of free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant.Figure 3 shows that the dielectric constant of the composite increases with increase in mass fraction of vinyl alcohol.

CONCLUSION

The possibility of use of polyvinyl alcohol and poly-1,2-β-D galactose to form a blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all the three parametersincreased with increase in mass fraction of vinyl alcohol. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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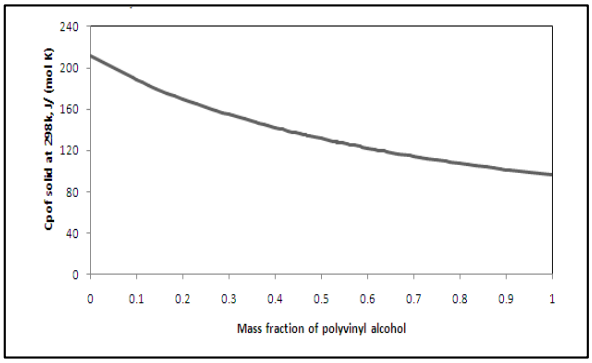

Figure 1. Change in heat capacity with mass fraction of vinyl alcohol

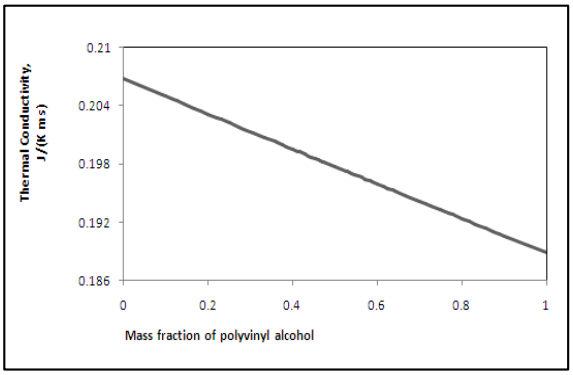

Figure 2. Change in thermal conductivity with mass fraction of vinyl alcohol

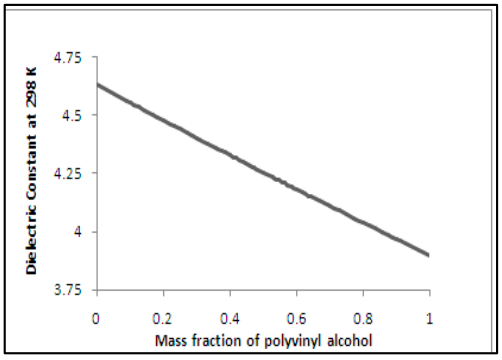

Figure 3. Change in dielectric constant with mass fraction of vinyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polyvinyl Alcohol and Poly-1,3-α-D-Galactose Composite

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ABSTRACT

A blend is a mixture of more than one component. The desired property of a blend is its homogeneity. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that all those parameters increased with increase in mass fraction of polyvinyl alcohol. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Thermal and dielectric , in silico, polyvinyl alcohol, poly-1,3-α-D-Galactose.

INTRODUCTION

Blends or composites are materials containing more than one component. The components do not lose their identity in the mixture. They combine and contribute to the property of the blend thereby improving the quality of the material. Development of a single material with the desired property involves significant research and time. A blend utilizes the advantages of different materials; mix them to get the desired property. Thus a blend saves time to develop a new material thereby reducing the cost of development of products with desired properties.Polymer blends can be made of two or more polymers, or fibres and polymer, or particles and polymer.

Nano material modified polymers paved the way to multi functional materials. Polymers coupled with carbon based (graphene, carbon nano-tube) nano-materials [1] have drawn attention. Biodegradable polymers- natural fiber composites [2] have been reported to enhance mechanical properties and water resistance. Researchers are working on fire retardant/fire proof materials [3]. There are reports of inorganic additives in polypropylene; that can enhance flame retardancywithout increasing the weight [4]. Researchers have emphasized on synthesis and production of lightweight composite materials having high strength important for enhancing fuel efficiency in the field of transportation [5]. There are applications of composites in structural Engineering due to high strength to weight ratio and resistance to corrosion. Thus, glass fiber reinforced polymers, latex polymer cementitious composites [6] were

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Among the various polymers, polyvinyl alcohol (PVA) is a promising material due to its high dielectric strength, easy film formation, adhesiveness and whose properties can be controlled by dopant concentrations [8, 9]. The film forming ability of PVA is widely used in packaging industry to form strong polymeric films. It is because of their high mechanical strength, environmental stability and easy processability [10]. On the other hand, PVA is non-toxic, semicrystalline, hydrophilic, biocompatible and easily soluble in water [11]. Researchers have found applications of glycopolymers (synthetic polymers containing pendant carbohydrate groups) in the separation and removal of toxins and bacteria, tumor cell recognition and glucose-responsive insulin delivery [12]. It has been found that biopolymer blends possess good thermal stability [13].This study is intended to identify the interaction of polyvinyl alcohol acid and Poly-1,3-α-D-Galactose to form blends.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systemes of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction.

Methodology: The structures of polyvinyl alcohol and poly-1,3-α-D-Galactose were fed to the synthia menu of Materials Studio. It was then run for different weight ractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polyvinyl alcohol on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polyvinyl alcohol and poly-1,3-α-D-Galactoseas potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated.

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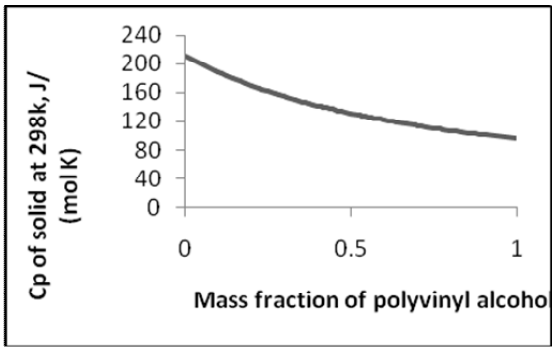

Figure 1. Change in heat capacity with mass fraction of vinyl alcohol

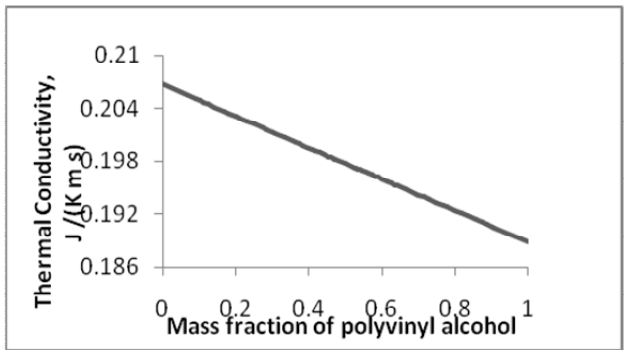

Figure 2. Change in thermal conductivity with mass fraction of vinyl alcohol

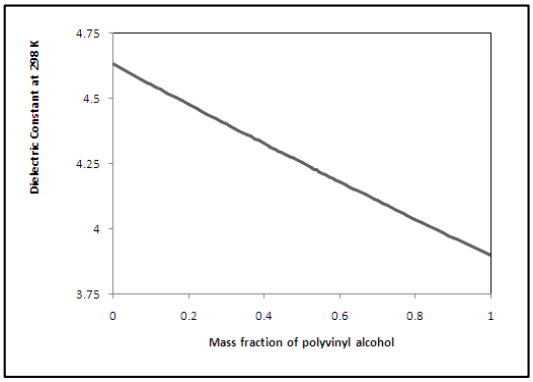

Figure 3. Change in dielectric constant with mass fraction of vi nyl alcohol

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RESEARCH ARTICLE

In silico Analysis of Thermal and Dielectric Properties of Polybiphenyl Dimethyl Carbonate and Polyether Sulfone Composite

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ABSTRACT

Preparing blend with two or more polymeric components is the easiest trend in developing hybrid materials with improved thermal and electrical properties. Depending on the compatibility of the constituting components, it may undergo in well mixing or phase separation within the hybrid blend. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant. The results indicated that only heat capacity of the hybrid material increases, while other properties like thermal conductivity and dielectric constant are decreased with increase of mass fraction of biphenyldimethyl carbonate. This study will help determine pairs without performing laboratory experiments saving materials, money and time.

Keywords: Hybrid Polymer, Thermal properties, Dielectric properties, Biovia,In-silico analysis

INTRODUCTION

The current age is essentially managing the improvement of existing one in all areas of science and technology. Polymeric blends are usually offered improved physical and chemical properties like thermal, mechanical, gas barrier and biodegradability [1]. These properties are the prime interest for the researchers to design best packaging material. Gas permeability is sometimes offered as essential criterion to design the polymer for biomedical and industrial utilization. For instance, polymers with high barrier properties, i.e. low permeability, are mandatory for food packaging applications to prevent loss of aroma, color and food-value and to slow down spoilage [2]. Apart from this food packaging application; there are lots of other applications which require the polymers to have high, low or tailored permeability like, filters and membranes for gas or liquid separation [3], protective coatings (e.g., paints and varnishes) [4], polymer coatings for controlled drug release [5] and water desalination [6].The permeability of liquids and gases through polymer membranes (plastic films) may be happened by either a temperature or pressure gradient, or by concentration gradient or external force field. The ‘‘solution-diffusion’’ mechanism is generally used to depict the pathway of gas permeation. It involvesthree steps. In the first step

absorption of small molecules is happened into the membrane at the side of higher gradient (concentration, pressure, etc). On the other hand, second step involves the molecular diffusion through the membrane and the final step is related to desorption of those molecules from the membrane at the opposite side of lower gradient. The gas permeability in a polymer is generally varied with the nature of polymer and permeates. It may be accounted due to various degree of crystallinity and porosity of the polymers along with surface functionality (hydrophilic/ hydrophobic groups).The main aim of combining polymeric materials is to achieve the desired quality of the material. Among various polymers, polybiphenyldimethylcarbonate (PC) is a widely used engineering plastics because of its physical and chemical properties like ductility, good thermal stability, excellent transparency, and high mechanical strength[7]. As a resultof these excellent properties, PC has been largely employed in electronic and electronic appliances along with automotive industry, having an annual production of 6 million tons. Recent report by Behboudiet. al. [8] shows thatPC is blended withpolyvinyl chloride (PVC)to preparethe ultrafiltration membrane for water purification. On the other hand, PC is also blended with poly(vinylidene fluoride) (PVDF) to prepare mechanically strong multicomponent nanocomposites with nanostructural reinforcement of graphenenanoplates, carbon nanotube, and organically modified montmorillonite [9].

In another recent report Wen et al. reinforced the graphene plates into blend of polybutyleneterethalate and polycarbonate [10] to obtain electrical and thermal conductive materials. The unique material, formed from the blend of PC with polystyrene is also reported to sense organic vapours with incorporation of multiwalled carbon nanotubes (MWCNTs) [11]. Polycarbonate blended polysulfone material is recently observed to have improved thermal and mechanical properties[12]. Therefore,investigationof blending compatibility of polycarbonate with other polymer is the urgent need of current research to develop advanced functional materials. All the above mentioned examples relied on laboratory experiments. Usually, preparation of homogeneous blend in wet-lab condition, requires huge time and wastage of materials which can be minimized by in-silico approach through material studio [13] of "Biovia" software.. In present context, we are focusing to optimize the homogeneous blend composition of polybiphrnyldimethylcarbonate (PC) with polyether sulfone (PES) in terms of gas permeability. Among various engineering polymers, polyether sulfone (PES) is a high-temperature sustaining thermoplastic polymer with striking strength and chemical stability from various organic solvents. It belongs to the polysulfone family and contains an aryl-SO_2 subunit in their long chain structures. Nonetheless, the inherent hydrophobic property of PES makes this material sensitive to membrane fouling, restricting its more extensive applications in membrane based water treatment. Due to high chemical stability it is also preferably used for gas separation in harsh environment.

To improve the gas separation efficiency of PES, a few investigations have been performed. In a report, Adib et al. [14] incorporated the nanostructural silica to improve the gas separation. However, blending of PES with other hydrophilic polymer is one of the easiest routes to improve the efficiency of the gas separation. In another report, Mannan et al. [15] investigated the gas-permeation behavior of glassy poly(vinyl acetate) (PVAc)–PES hybrid films and PSF–PES film. Interestingly, it is found that the gas permeation properties of hybrid PSF–PES film is remain unaltered as compared to the properties of polyether sulfone. However on account of the PES–PVAc hybrid polymer, low selectivity was observed for gas separation and may be accounted as the phase separation in their blend. Kamal et al. [16] revealed that the blend with elastomers (like polydimethylsiloxane) leads to the improved gas permeation properties of the polydimethylsiloxane–PES hybrid. Akbarian et al.[17] prepared the PES based blend membranes for CO_2 gas separation with inclusion polyethylene glycol (PEG) as second polymer. Therefore, the present in-silico approach of blend analysis between poly(biphenyl dimethyl carbonate) (PC) and polyether sulfone (PES) may be utilized to optimize the composition to fabricate desirable functional materials with some improved physical and chemical properties.

MATERIALS AND METHODS

Software Used: Materials studio module of Biovia software (Dassault Systems of France) was used for analysis. The software utilizes machine learning techniques and standard algorithms to predict the level of interaction

Methodology: The structures of polybiphenyl dimethyl carbonate and polyether sulfone were fed to the synthia menu of Materials Studio. It was then run for different weight fractions of the components. Different properties of the composite were displayed in a tabular form. The values were used to plot graphs to identify the effect of weight fraction of polybiphenyl dimethyl carbonate on the mechanical properties of the composite.

RESULTS AND DISCUSSION

In this work the use of polybiphenyl dimethyl carbonateand polyether sulfoneas potential components of a composite was analyzed using Biovia Materials Studio. BIOVIA Materials Studio Synthia uses pre-defined correlations (advanced quantitative structure-property relationships) to evaluate a wide range of polymer properties. Group additive methods were used for many years to predict the properties of polymers as well as small molecules. These methods are extremely fast and easy to use. Consequently, they are of greatest utility when a rapid estimate of a property is required without a detailed understanding of the atomistic interactions that give rise to it. However, the principal shortcoming of these methods is their dependence upon a database of group contributions. Thus, if a polymer contains a group for which the group contribution cannot be estimated, then the property of that polymer cannot be calculated. To overcome this limitation, the method implemented in Synthia uses topological information about polymers in the predictive correlations. The connectivity indices derived from graph theory are employed. Thus, no database of group contributions is required and properties may be predicted for any polymer composed of any combination of the following nine elements: carbon, hydrogen, nitrogen, oxygen, silicon, sulfur, fluorine, chlorine, bromine.

Heat Capacity: It is the amount of heatrequired to raise the temperature of one unit weight of a substance by 1°C without change of phase.Figure 1 shows that the heat capacity (Cp) of the composite increases linearly with increase in mass fraction of biphenyl dimethyl carbonate.

Thermal Conductivity: It indicates the correlation between heat flux per unit area and temperature gradient.It refers to the intrinsic ability of a material to transfer heat.Figure 2 shows that the thermal conductivity of the composite decreases linearly with increase in mass fraction of biphenyl dimethyl carbonate.

Dielectric Constant: It is defined as the ratio of the electric permeability of the material to the electric permeability of free space. As the dielectric constant increases, the electric flux density increases, while all other factors are maintained constant.Figure 3 shows that the dielectric constants of the composite decreases with increase in mass fraction of biphenyl dimethyl carbonate.

CONCLUSION

The possibility of use of poly (biphenyl dimethyl carbonate) and polyether sulfone to form a blend was explored using Biovia Materials Studio. The composition of the blend was analyzed with respect to heat capacity, thermal conductivity and dielectric constant.The results indicated that only heat capacity of the hybrid material increases, while other properties like thermal conductivity and dielectric constant are decreased with increase of mass fraction of biphenyl dimethyl carbonate. Usually components for a blend are identified experimentally. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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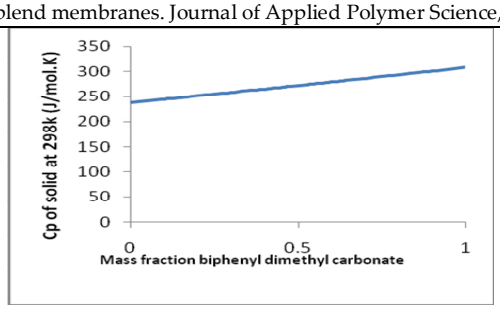

Figure 1. Change in heat capacity with mass fraction of biphenyl dimethyl carbonate

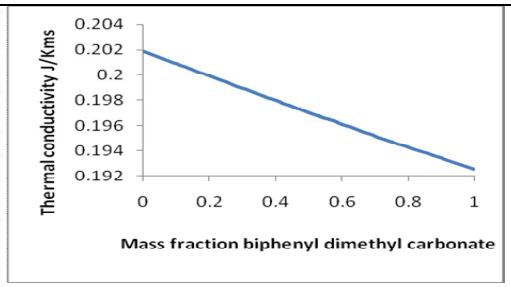

Figure 2. Change in thermal conductivity with mass fraction of biphenyl dimethyl carbonate

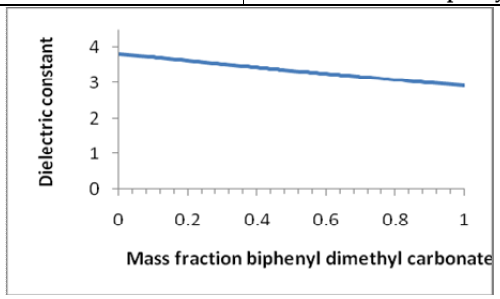

Figure 3. Change in dielectric constant with mass fraction of biphenyl dimethyl carbonate

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Clc1nc(Cl)nc(n1)N2CCCc3ccccc23 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code Clc1nc(Cl)nc(n1)N2CCCc3ccccc23.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral

enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code Clc1nc(Cl)nc(n1)N2CCCc3ccccc23. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code Clc1nc(Cl)nc(n1)N2CCCc3ccccc23. This in silico study will help determine components of a blend without performing laboratory experiments saving materials, money and time.

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2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	Clc1nc(Cl)nc(n1)N2CCCc3ccccc23	28.254200000000001	20.476199999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Nc1cc(CCC(=O)O)ccc1O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code Nc1cc(CCC(=O)O)ccc1O.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

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MATERIALS AND METHODS

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code Nc1cc(CCC(=O)O)ccc1O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code Nc1cc(CCC(=O)O)ccc1O.

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2	Pharmacophore	Nc1cc(CCC(=O)O)ccc1O	21.253499999999999	18.770700000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CN(C)C[C@H](O)COCc1occc1 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CN(C)C[C@H](O)COCc1occc1.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

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MATERIALS AND METHODS

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CN(C)C[C@H](O)COCc1occc1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CN(C)C[C@H](O)COCc1occc1	17.584299999999999	20.688099999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC(=O)c1cc2CCCCc2c(O)c1O (SMILES)

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ABSTRACT

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MATERIALS AND METHODS

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RESULTS AND DISCUSSION

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CC(=O)c1cc2CCCCc2c(O)c1O.

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2	Pharmacophore	CC(=O)c1cc2CCCCc2c(O)c1O	18.932200000000002	20.004999999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore C[C@H]1C[C@H](CC(C)(C)C1)OC=O (SMILES)

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2	Pharmacophore	C[C@H]1C[C@H](CC(C)(C)C1)OC=O	12.3019	18.9282

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore C[C@@H]1CC(C)(C)N(CCO)c2cc(C)ccc12 (SMILES)

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MATERIALS AND METHODS

Methodology

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used

CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code C[C@@H]1CC(C)(C)N(CCO)c2cc(C)ccc12. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code C[C@@H]1CC(C)(C)N(CCO)c2cc(C)ccc12.

REFERENCES

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	C[C@@H]1CC(C)(C)N(CCO)c2cc(C)ccc12	19.434000000000001	26.313700000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CON1[C@@H]2CCCC[C@@H]2N(OC)C(=O)C1=O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CON1[C@@H]2CCCC[C@@H]2N(OC)C(=O)C1=O.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CON1[C@@H]2CCCC[C@@H]2N(OC)C(=O)C1=O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CON1[C@@H]2CCCC[C@@H]2N(OC)C(=O)C1=O	10.6059	20.8643

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC1(C)N(O)[C@H](NC1=S)c2ccccc2 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC1(C)N(O)[C@H](NC1=S)c2ccccc2.

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CC1(C)N(O)[C@H](NC1=S)c2ccccc2. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CC1(C)N(O)[C@H](NC1=S)c2ccccc2	14.007999999999999	19.980799999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore NNC(=O)C(=O)NC1CCCCC1 (SMILES)

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ABSTRACT

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Keywords: Corona, Virus, Docking, Pharmacophore

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"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code NNC(=O)C(=O)NC1CCCCC1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	NNC(=O)C(=O)NC1CCCCC1	14.4819	21.3947

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CCOC(=O)CNC(C)(C)C (SMILES)

Ramesh Sahu

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ABSTRACT

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore COC(=O)CS[C@H](C)CC(=O)OC (SMILES)

Debajani Tripathy

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RESEARCH ARTICLE

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B. Barik

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Table 1. Results of CDOCK

SL NO	Type	Compound	"-C DOCKER ENERGY"	"-C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	COC(=O)[C@H]1SCC(=O)[C@H]1C(=O)OC	17.770299999999999	17.947900000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Cc1ccc(C)n1CC2CCNCC2 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code Cc1ccc(C)n1CC2CCNCC2.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code Cc1ccc(C)n1CC2CCNCC2. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code Cc1ccc(C)n1CC2CCNCC2.

REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). (2020).
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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	Cc1ccc(C)n1CC2CCNCC2	16.4587	21.269300000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Oc1cc2CCN=Cc2cc1O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code Oc1cc2CCN=Cc2cc1O.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology:"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the

viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code Oc1cc2CCN=Cc2cc1O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code Oc1cc2CCN=Cc2cc1O.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	Oc1cc2CCN=Cc2cc1O	10.4091	13.5372

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CCOC(=O)C(=O)N1CCC(CC1)NC(=O)C2CCCCC2 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CCOC(=O)C(=O)N1CCC(CC1)NC(=O)C2CCCCC2.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CCOC(=O)C(=O)N1CCC(CC1)NC(=O)C2CCCCC2. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CCOC(=O)C(=O)N1CCC(CC1)NC(=O)C2CCCCC2.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CCOC(=O)C(=O)N1CCC(CC1)NC(=O)C2CCCCC2	15.589399999999999	29.918099999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore C[N+](C)(C)CC(=O)c1ccc2OCCOc2c1 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code C[N+](C)(C)CC(=O)c1ccc2OCCOc2c1.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code C[N+](C)(C)CC(=O)c1ccc2OCCOc2c1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code C[N+](C)(C)CC(=O)c1ccc2OCCOc2c1.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	C[N+](C)(C)CC(=O)c1ccc2OCCOc2c1	12.1783	24.519200000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore NN1C=Cc2ccccc2C1=N (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code NN1C=Cc2ccccc2C1=N.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

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MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code NN1C=Cc2ccccc2C1=N. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code NN1C=Cc2ccccc2C1=N.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"-C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	NN1C=Cc2ccccc2C1=N	10.348800000000001	13.4267

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC1(C)SC(C)(C)N(C=O)[C@H]1C(=O)O (SMILES)

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CONCLUSIONS

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CC1(C)SC(C)(C)N(C=O)[C@H]1C(=O)O	14.6988	18.352

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CCC(=O)Oc1sc(NCCc2ccccc2)[n+](C)c1C (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CCC(=O)Oc1sc(NCCc2ccccc2)[n+](C)c1C.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CCC(=O)Oc1sc(NCCc2ccccc2)[n+](C)c1C. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CCC(=O)Oc1sc(NCCc2ccccc2)[n+](C)c1C.

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1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CCC(=O)Oc1sc(NCCc2ccccc2)[n+](C)c1C	29.0166	33.312399999999997

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Cc1ccc(O)c(c1)C(=O)NO (SMILES)

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ABSTRACT

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2	Pharmacophore	Cc1ccc(O)c(c1)C(=O)NO	12.889799999999999	16.132000000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CCc1c(C(=O)OC)c2cc(O)ccc2n1Cc3ccccc3 (SMILES)

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2	Pharmacophore	CCc1c(C(=O)OC)c2cc(O)ccc2n1Cc3ccccc3	23.2593	28.513300000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CCOC(=O)Cc1c(C)[nH]c2ccc(cc12)C(C)C (SMILES)

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Received: 23 Mar 2020 Revised: 25 Apr 2020 Accepted: 28 May 2020

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore O=C1CCCCCN1SSN2CCCCCC2=O (SMILES)

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Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CSC[C@H](O)CN1N=C(O)C(=C(Cl)C1=O)Cl. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CSC[C@H](O)CN1N=C(O)C(=C(Cl)C1=O)Cl.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CSC[C@H](O)CN1N=C(O)C(=C(Cl)C1=O)Cl	14.1793	22.852900000000002

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC(C)(C)c1cc2C(=O)CC(C)(C)Oc2c(O)c1O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(C)(C)c1cc2C(=O)CC(C)(C)Oc2c(O)c1O.

Keywords: Corona, Virus, Docking, Pharmacophore

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"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral

enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

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Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CC(C)(C)c1cc2C(=O)CC(C)(C)Oc2c(O)c1O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC(C)c1cc(SC#N)c(C)cc1O (SMILES)

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RESEARCH ARTICLE

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R. Mishra

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2	Pharmacophore	CCOC(=O)C(N(C)C)C(=O)OCC	19.451899999999998	23.532499999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Cc1cc(C)c(CC(=O)O)c(C)c1 (SMILES)

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RESEARCH ARTICLE

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	OC(=O)[C@@H]1CS[C@@H](N1)c2ccc(cc2)[C@@H]3N[C@@H](CS3)C(=O)O	14.885300000000001	27.721699999999998

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CN1C(=O)O[C@H](C1=O)c2ccccc2 (SMILES)

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Received: 25 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CN1C(=O)O[C@H](C1=O)c2ccccc2.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CN1C(=O)O[C@H](C1=O)c2ccccc2. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Cn1cnc(C(=O)O)c1C(=O)O (SMILES)

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Received: 23 Mar 2020 Revised: 25 Apr 2020 Accepted: 28 May 2020

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1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	Cn1cnc(C(=O)O)c1C(=O)O	12.312900000000001	15.085800000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC(C)(C)\C(=C\C(=O)C(C)(C)C)\[O-] (SMILES)

Nibedita Nayak

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Received: 24 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

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Keywords: Corona, Virus, Docking, Pharmacophore

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MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive

value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CC(C)(C)\C(=C\C(=O)C(C)(C)C)\[O-]. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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2	Pharmacophore	CC(C)(C)\C(=C\C(=O)C(C)(C)C)\[O-]	22.503	28.0259

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Cc1cc(C[NH+]2CCOCC2)c(C)cc1O (SMILES)

Nibedita Nayak

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Received: 25 Mar 2020 Revised: 27 Apr 2020 Accepted: 28 May 2020

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2	Pharmacophore	Cc1cc(C[NH+]2CCOCC2)c(C)cc1O	10.5937	20.4923

4.

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CCOC(=O)[C@@H]1C[NH2+]CCC1=O (SMILES)

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Received: 26 Mar 2020 Revised: 27 Apr 2020 Accepted: 28 May 2020

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R. Mishra and Nibedita Nayak*

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CCOC(=O)[C@H]1CC[N@@H+](Cc2ccccc2)CC1=O (SMILES)

Nibedita Nayak

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CCOC(=O)[C@H]1CC[N@@H+](Cc2ccccc2)CC1=O.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CCOC(=O)[C@H]1CC[N@@H+](Cc2ccccc2)CC1=O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CCOC(=O)[C@H]1CC[N@@H+](Cc2ccccc2)CC1=O.

REFERENCES

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CCOC(=O)[C@H]1CC[N@@H+](Cc2ccccc2)CC1=O	24.0045	27.064699999999998

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore [O-]C(=O)C(=O)Cc1ccccc1 (SMILES)

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2	Pharmacophore	[O-]C(=O)C(=O)Cc1ccccc1	12.0115	16.626799999999999

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1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	C[C@@H]([C@H](O)c1ccccc1)[NH+](C)C	10.497400000000001	19.756599999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Oc1cc([O-])nc2ccccc12 (SMILES)

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Keywords: Corona, Virus, Docking, Pharmacophore

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MATERIALS AND METHODS

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1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	Oc1cc([O-])nc2ccccc12	10.7895	20.793800000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore OC(=O)C[NH2+]Cc1ccccc1 (SMILES)

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2	Pharmacophore	OC(=O)C[NH2+]Cc1ccccc1	21.724599999999999	18.907699999999998

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CC(C)(C)[C@H](NC=O)C(=O)O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CC(C)(C)[C@H](NC=O)C(=O)O.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CC(C)(C)[C@H](NC=O)C(=O)O	13.558199999999999	14.295400000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore COC(=O)[C@H](CC(=O)O)C(C)C (SMILES)

Subrata Sarangi

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Received: 25 Mar 2020 Revised: 27 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code COC(=O)[C@H](CC(=O)O)C(C)C.

Keywords: Corona, Virus, Docking, Pharmacophore

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4.

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RESEARCH ARTICLE

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Subrata Sarangi

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2	Pharmacophore	C[NH+]1CCN(Cc2ccccc2)CC1	10.879200000000001	21.692499999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC(C)[C@@H]1CC[C@@H](C)C[C@H]1OC(=O)C(O)O (SMILES)

R. Mishra

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RESEARCH ARTICLE

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R. Mishra

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CC(=O)Nc1ccc(cc1)S(=O)(=O)NC2(CCCCC2)C(=O)O	24.021799999999999	29.2897

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Nc1ccc2Cc3ccc(N)cc3S(=O)(=O)c2c1 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code Nc1ccc2Cc3ccc(N)cc3S(=O)(=O)c2c1.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code Nc1ccc2Cc3ccc(N)cc3S(=O)(=O)c2c1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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RESEARCH ARTICLE

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2	Pharmacophore	OC(=O)CCc1ncccn1	23.2316	16.725100000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC(=O)NC(NC(=O)C)C(=O)c1ccccc1 (SMILES)

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2	Pharmacophore	CC(=O)NC(NC(=O)C)C(=O)c1ccccc1	23.604299999999999	22.331399999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore OC(=O)CCC(=O)N(Nc1ccccc1)c2ccccc2 (SMILES)

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Keywords: Corona, Virus, Docking, Pharmacophore

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	OC(=O)CCC(=O)N(Nc1ccccc1)c2ccccc2	21.036300000000001	27.391500000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Cc1oc(C[N+](C)(C)C)cc1 (SMILES)

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RESULTS AND DISCUSSION

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RESEARCH ARTICLE

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Keywords: Corona, Virus, Docking, Pharmacophore

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Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CN(C)CCS[C@H](CO)c1ccccc1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC1(C)OC(=O)C[C@H]1C(=O)O (SMILES)

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RESEARCH ARTICLE

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CC(C)(C)[C@H](O)C(=O)C(C)(C)C.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CC(C)(C)[C@H](O)C(=O)C(C)(C)C	12.299099999999999	17.765899999999998

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore COC(=O)[C@](C)(N)Cc1ccc(O)cc1 (SMILES)

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Received: 23 Mar 2020 Revised: 24 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code COC(=O)[C@](C)(N)Cc1ccc(O)cc1.

Keywords: Corona, Virus, Docking, Pharmacophore

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MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code COC(=O)[C@](C)(N)Cc1ccc(O)cc1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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2	Pharmacophore	CC(C)C(=O)OC[C@H](C)c1ccccc1	22.267199999999999	21.166

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RESEARCH ARTICLE

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2	Pharmacophore	CCOC(=N)c1ccc(O)cc1	10.8101	12.917199999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CN1CCCN2CCCN=C12 (SMILES)

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Received: 24 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CN1CCCN2CCCN=C12.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3].The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CN1CCCN2CCCN=C12. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CN1CCCN2CCCN=C12.

REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). (2020).
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3. D. Das, S. Das, M. Pandey, D. Bhattacharyay. "In silico Analysis of Phytochemicals from Mucuna pruriens (L.) DC against Mycobacterium tuberculosis Causing Tuberculosis", European Journal of Medicinal Plants (2020) 31(4), 19-24.

Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CN1CCCN2CCCN=C12	11.0585	14.441800000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore O=C1N[C@H](CO1)c2ccccc2 (SMILES)

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Received: 25 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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Keywords: Corona, Virus, Docking, Pharmacophore

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MATERIALS AND METHODS

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RESULTS AND DISCUSSION

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	O=C1N[C@H](CO1)c2ccccc2	11.218299999999999	15.6495

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC(=O)NC1=NC(=O)NC=C1 (SMILES)

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Received: 24 Mar 2020 Revised: 27 Apr 2020 Accepted: 28 May 2020

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Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CC(=O)NC1=NC(=O)NC=C1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CC(=O)NC1=NC(=O)NC=C1	11.0989	14.1234

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CN(C)Cc1oc(CO)cc1 (SMILES)

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ABSTRACT

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Keywords: Corona, Virus, Docking, Pharmacophore

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CN(C)Cc1oc(CO)cc1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CN(C)Cc1oc(CO)cc1	14.794600000000001	14.9284

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC(=O)O[C@@H]1CS[C@H](O1)C(=O)O (SMILES)

Prativa Satpathy

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ABSTRACT

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Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

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MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CC(=O)O[C@@H]1CS[C@H](O1)C(=O)O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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CONCLUSIONS

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore NS(=O)(=O)c1cc(C(=O)O)c(NCc2ccccc2)cc1Cl (SMILES)

Sujata Acharya

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Received: 23 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore COc1cc2C[NH2+][C@@H](Cc2cc1OC)C(=O)O (SMILES)

Asha rani Dalai

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Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code COc1cc2C[NH2+][C@@H](Cc2cc1OC)C(=O)O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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CONCLUSIONS

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC(=O)CCc1c(C)c(OC(=O)C)c(C)c(C)c1OC(=O)C (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(=O)CCc1c(C)c(OC(=O)C)c(C)c(C)c1OC(=O)C.

Keywords: Corona, Virus, Docking, Pharmacophore

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC(C)C1=CC(=O)Oc2c3CCCN4CCCc(cc12)c34 (SMILES)

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ABSTRACT

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CC(C)C1=CC(=O)Oc2c3CCCN4CCCc(cc12)c34.

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1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CC(C)C1=CC(=O)Oc2c3CCCN4CCCc(cc12)c34	12.2684	24.5715

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RESEARCH ARTICLE

Deactivation of 6VWW enzyme of corona by pharmacophore COC(=O)N1CCC[C@H]1C(O)(c2ccccc2)c3ccccc3 (SMILES)

S. Naik

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ABSTRACT

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Keywords: Corona, Virus, Docking, Pharmacophore

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1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	COC(=O)N1CCC[C@H]1C(O)(c2ccccc2)c3ccccc3	10.703900000000001	24.714500000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore OC(=O)c1[nH]c(C(=O)O)c2OCCOc12 (SMILES)

Monalisa Joshi

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ABSTRACT

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RESEARCH ARTICLE

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Lokanath Meher

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore COc1ccc(C[C@@H]2NC[C@@H](O)[C@@H]2OC(=O)C)cc1 (SMILES)

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code COc1ccc(C[C@@H]2NC[C@@H](O)[C@@H]2OC(=O)C)cc1. Positive values of "-CDOCK Energy and - CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code COc1ccc(C[C@@H]2NC[C@@H](O)[C@@H]2OC(=O)C)cc1.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	COc1ccc(C[C@@H]2NC[C@@H](O)[C@@H]2OC(=O)C)cc1	10.3231	32.235700000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore ONS(=O)(=O)c1ccccc1 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code ONS(=O)(=O)c1ccccc1.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

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Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code ONS(=O)(=O)c1ccccc1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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2	Pharmacophore	ONS(=O)(=O)c1ccccc1	10.3704	13.8238

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore OC[C@@H](O)COc1ccc(Cc2ccc(OC[C@H](O)CO)cc2)cc1 (SMILES)

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ABSTRACT

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MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code OC[C@@H](O)COc1ccc(Cc2ccc(OC[C@H](O)CO)cc2)cc1. Positive values of "-CDOCK Energy and - CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code OC[C@@H](O)COc1ccc(Cc2ccc(OC[C@H](O)CO)cc2)cc1.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	OC[C@@H](O)COc1ccc(Cc2ccc(OC[C@H](O)CO)cc2)cc1	14.243499999999999	31.9404

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC(=O)C1=C([O-])C=C(C)OC1=O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(=O)C1=C([O-])C=C(C)OC1=O.

Keywords: Corona, Virus, Docking, Pharmacophore

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MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CC(=O)C1=C([O-])C=C(C)OC1=O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CC(=O)C1=C([O-])C=C(C)OC1=O	13.3398	22.8079

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CCOC(OCC)n1ccnc1 (SMILES)

G. Mishra

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ABSTRACT

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1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CCOC(OCC)n1ccnc1	16.2576	13.707700000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore COc1cc(cc(OC)c1O)C(=O)C (SMILES)

Jyoti Rath

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1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC1(C)O[C@@H](CC(=O)O)C(=O)O1 (SMILES)

Namita Panda

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CC1(C)O[C@@H](CC(=O)O)C(=O)O1	17.614799999999999	15.8773

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore OC[C@H](Cc1cccc(O)c1)[C@H](CO)Cc2cccc(O)c2 (SMILES)

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Received: 23 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code OC[C@H](Cc1cccc(O)c1)[C@H](CO)Cc2cccc(O)c2.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code OC[C@H](Cc1cccc(O)c1)[C@H](CO)Cc2cccc(O)c2. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code OC[C@H](Cc1cccc(O)c1)[C@H](CO)Cc2cccc(O)c2.

REFERENCES

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	OC[C@H](Cc1cccc(O)c1)[C@H](CO)Cc2cccc(O)c2	22.8142	32.702399999999997

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC1=CC(=O)Oc2cc(OC(=O)c3ccc(NC(=N)N)cc3)ccc12 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC1=CC(=O)Oc2cc(OC(=O)c3ccc(NC(=N)N)cc3)ccc12.

Keywords: Corona, Virus, Docking, Pharmacophore

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MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CC1=CC(=O)Oc2cc(OC(=O)c3ccc(NC(=N)N)cc3)ccc12. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CC1=CC(=O)Oc2cc(OC(=O)c3ccc(NC(=N)N)cc3)ccc12.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	CC1=CC(=O)Oc2cc(OC(=O)c3ccc(NC(=N)N)cc3)ccc12	14.1409	27.9071

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC(C)[C@H]1CC[C@H](C)C[C@@H]1OCC(=O)O (SMILES)

C. Tripathy

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Received: 25 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(C)[C@H]1CC[C@H](C)C[C@@H]1OCC(=O)O.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CC(C)[C@H]1CC[C@H](C)C[C@@H]1OCC(=O)O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	CC(C)[C@H]1CC[C@H](C)C[C@@H]1OCC(=O)O	14.6144	22.424299999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CCN1C=C(C(=O)[O-])C(=O)c2ccc(C)nc12 (SMILES)

D. Tripaty

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Received: 26 Mar 2020 Revised: 27 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

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Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

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MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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RESULTS AND DISCUSSION

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of COrona by Pharmacophore N[C@@H](CSc1nccs1)C(=O)O (SMILES)

R. Mishra

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Received: 25 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Nc1ccc(cc1)S(=O)(=O)[N-]c2nccs2 (SMILES)

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CN1C(=O)N=C([O-])c2c1ncn2C (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CN1C(=O)N=C([O-])c2c1ncn2C.

Keywords: Corona, Virus, Docking, Pharmacophore

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"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

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Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CN1C(=O)N=C([O-])c2c1ncn2C. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CN1C(=O)N=C([O-])c2c1ncn2C.

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore COc1ccc2C(=CC(=O)Oc2c1)CC(=O)ON3C(=O)CCC3=O (SMILES)

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Received: 25 Mar 2020 Revised: 27 Apr 2020 Accepted: 28 May 2020

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CC(=O)[C@@H]1C(=O)OC(=CC1=O)C. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials.

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Oc1ccc(O)c(Cc2nc3ccccc3s2)c1 (SMILES)

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Keywords: Corona, Virus, Docking, Pharmacophore

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RESEARCH ARTICLE

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	C[C@H]1CCCC[C@@]12NC(=O)NC2=O	11.6783	18.895800000000001

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RESEARCH ARTICLE

Deactivation of 6VWW enzyme of corona by pharmacophore CN1C(=O)N(C)c2ncn(Cc3ncc[nH]3)c2C1=O (SMILES)

R. Mishra

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Received: 24 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CN1C(=O)N(C)c2ncn(Cc3ncc[nH]3)c2C1=O.

Keywords: Corona, Virus, Docking, Pharmacophore

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Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CN1C(=O)N(C)c2ncn(Cc3ncc[nH]3)c2C1=O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

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RESEARCH ARTICLE

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CCOC(=O)CCc1ccc(\C=C\C(=O)OCC)[nH]1 (SMILES)

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Cc1c(CO)sc[n+]1Cc2ccccc2 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CN(C)Cc1c(C)[nH]c(C)c1CN(C)C.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CN(C)Cc1c(C)[nH]c(C)c1CN(C)C. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CN(C)Cc1c(C)[nH]c(C)c1CN(C)C.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	CN(C)Cc1c(C)[nH]c(C)c1CN (C)C	22.197900000000001	20.366599999999998

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RESEARCH ARTICLE

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2	Pharmacophore	CNC(=O)CN1C(=O)CCC1=O	20.040900000000001	18.845800000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CN1CCN(CC1)C(=O)CN2N=C(C=CC2=O)c3ccc(C)cc3 (SMILES)

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2	Pharmacophore	CN1CCN(CC1)C(=O)CN2N=C(C=CC2=O)c3 ccc(C)cc3	17.246700000000001	30.828399999999998

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore NC(=O)c1ccc(NCC(=O)O)cc1 (SMILES)

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Keywords: Corona, Virus, Docking, Pharmacophore

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2	Pharmacophore	NC(=O)c1ccc(NCC(=O)O)cc1	19.8629	20.679600000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Oc1cc(O)c(C(=O)Cc2ccc(F)cc2)c(O)c1 (SMILES)

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Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code Cc1ccc2[C@H](CO)c3ccccc3[C@H](CO)c2c1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code Cc1ccc2[C@H](CO)c3ccccc3[C@H](CO)c2c1.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	Cc1ccc2[C@H](CO)c3ccccc3[C@H](CO)c2c1	18.211099999999998	23.828199999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore OC(=O)\C=C\C1=CC(=O)C(=CO1)OCc2ccccc2 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code OC(=O)\C=C\C1=CC(=O)C(=CO1)OCc2ccccc2.

Keywords: Corona, Virus, Docking, Pharmacophore

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore O=C1NC(=O)C2=NC=CNC2=N1 (SMILES)

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1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	O=C1NC(=O)C2=NC=CNC2=N1	10.181900000000001	15.5959

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore C[C@H](C(=O)C)n1c(CN2CCOCC2)nc3N(C)C(=O)N(C)C(=O)c13 (SMILES)

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Keywords: Corona, Virus, Docking, Pharmacophore

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2	Pharmacophore	C[C@H](C(=O)C)n1c(CN2CCOCC2)nc3N(C)C(=O)N(C)C(=O)c13	20.107500000000002	32.198

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CN1C(=O)NC(=O)c2[nH]c(nc12)N3CCN(CCO)CC3 (SMILES)

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ABSTRACT

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Keywords: Corona, Virus, Docking, Pharmacophore

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The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CN1C(=O)NC(=O)c2[nH]c(nc12)N3CCN(CCO)CC3.

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RESEARCH ARTICLE

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Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code COc1ccc(\C(=N\O)\c2ccc(N)cc2)c(OC)c1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code COc1ccc(\C(=N\O)\c2ccc(N)cc2)c(OC)c1.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	COc1ccc(\C(=N\O)\c2ccc(N)cc2)c(OC)c1	16.013300000000001	29.335799999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CCOc1ccc(C(=O)NN)c(O)c1 (SMILES)

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Received: 23 Mar 2020 Revised: 27 Apr 2020 Accepted: 28 May 2020

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"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CCOc1ccc(C(=O)NN)c(O)c1.

Keywords: Corona, Virus, Docking, Pharmacophore

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"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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RESEARCH ARTICLE

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore Nc1c(Br)cc(Br)cc1CN[C@@H]2CC[C@@H](O)CC2 (SMILES)

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	C[C@H](C[N+](C)(C)C)OC(=O)N	15.347300000000001	17.295300000000001

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CC(C)(C)NC[C@H](O)c1cc(Cl)c(N)c(Cl)c1 (SMILES)

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Received: 24 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(C)(C)NC[C@H](O)c1cc(Cl)c(N)c(Cl)c1.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology:"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CC(C)(C)NC[C@H](O)c1cc(Cl)c(N)c(Cl)c1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code CC(C)(C)NC[C@H](O)c1cc(Cl)c(N)c(Cl)c1.

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2	Pharmacophore	CC(C)(C)NC[C@H](O)c1cc(Cl)c(N)c(Cl)c1	19.1311	23.2818

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore C[N+](C)(C)CCOC(=O)Oc1ccc2ccccc2c1 (SMILES)

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Received: 23 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

Abstract

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Keywords: Corona, Virus, Docking, Pharmacophore

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MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the

viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3].The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code C[N+](C)(C)CCOC(=O)Oc1ccc2ccccc2c1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	myricetin	28.233799999999999	29.700299999999999
2	Pharmacophore	C[N+](C)(C)CCOC(=O)Oc1ccc2ccccc2c1	12.4948	31.5425

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore CCc1cccc2c3CCO[C@@](CC)(CC(=O)O)c3[nH]c12 (SMILES)

Sasi Bhusana Padhi

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Received: 23 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CCc1cccc2c3CCO[C@@](CC)(CC(=O)O)c3[nH]c12.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

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MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with myricetin of orange plant. The important enzyme of corona virus chosen was 6VWW.

RESULTS AND DISCUSSION

Table 1 shows that myricetin can block 6VWW enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6VWW. The pharmacophore had SMILES code CCc1cccc2c3CCO[C@@](CC)(CC(=O)O)c3[nH]c12. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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2	Pharmacophore	CCc1cccc2c3CCO[C@@](CC)(CC(=O)O)c3 [nH]c12	15.886799999999999	26.258099999999999

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RESEARCH ARTICLE

Deactivation of 6VWW Enzyme of Corona by Pharmacophore NC(=O)OC1(CCCCC1)C#C (SMILES)

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Received: 25 Mar 2020 Revised: 27 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6VWW enzyme of corona virus was identified. A pharmacophore equivalent to myricetin obtained from orange plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code NC(=O)OC1(CCCCC1)C#C.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

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RESULTS AND DISCUSSION

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CONCLUSIONS

The results suggested that myricetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6VWW enzyme of corona virus had SMILES code NC(=O)OC1(CCCCC1)C#C.

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore Nc1cc(CCC(=O)O)ccc1O (SMILES)

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Received: 25 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6W4B enzyme of corona virus was identified. A pharmacophore equivalent to vanillic acid obtained from cocoa plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code Nc1cc(CCC(=O)O)ccc1O.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with vanillic acid of cocoa plant. The important enzyme of corona virus chosen was 6W4B.

RESULTS AND DISCUSSION

Table 1 shows that vanillic acid can block 6W4B enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6W4B. The pharmacophore had SMILES code Nc1cc(CCC(=O)O)ccc1O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	Nc1cc(CCC(=O)O)ccc1O	25.978000000000002	24.193100000000001

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RESEARCH ARTICLE

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2	Pharmacophore	C=CCN1CCS(=O)(=O)CC1	11.386799999999999	19.3704

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"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6W4B enzyme of corona virus was identified. A pharmacophore equivalent to vanillic acid obtained from cocoa plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CCOC(=O)CNC(C)(C)C.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with vanillic acid of cocoa plant. The important enzyme of corona virus chosen was 6W4B.

RESULTS AND DISCUSSION

Table 1 shows that vanillic acid can block 6W4B enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6W4B. The pharmacophore had SMILES code CCOC(=O)CNC(C)(C)C. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that vanillic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6W4B enzyme of corona virus had SMILES code CCOC(=O)CNC(C)(C)C.

REFERENCES

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	CCOC(=O)CNC(C)(C)C	17.648499999999999	21.389600000000002

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore Oc1cc2CCN=Cc2cc1O (SMILES)

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Received: 24 Mar 2020 Revised: 25 Apr 2020 Accepted: 28 May 2020

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2	Pharmacophore	Oc1cc2CCN=Cc2cc1O	16.456	19.889700000000001

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2	Pharmacophore	NN1C=Cc2ccccc2C1=N	16.2318	21.117899999999999

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RESEARCH ARTICLE

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Sasi Bhusana Padhi

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2	Pharmacophore	Cc1ccc(O)c(c1)C(=O)NO	19.8888	24.4451

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore C[C@H](SCS[C@H](C)C(=O)O)C(=O)O (SMILES)

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RESEARCH ARTICLE

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Table 1 shows that vanillic acid can block 6W4B enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6W4B. The pharmacophore had SMILES code CN1C(=O)O[C@H](C1=O)c2ccccc2. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that vanillic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6W4B enzyme of corona virus had SMILES code CN1C(=O)O[C@H](C1=O)c2ccccc2.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	CN1C(=O)O[C@H](C1=O)c2ccccc2	17.309999999999999	23.8645

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore Cn1cnc(C(=O)O)c1C(=O)O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6W4B enzyme of corona virus was identified. A pharmacophore equivalent to vanillic acid obtained from cocoa plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code Cn1cnc(C(=O)O)c1C(=O)O.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	Cn1cnc(C(=O)O)c1C(=O)O	18.2363	23.107199999999999

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RESEARCH ARTICLE

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RESULTS AND DISCUSSION

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CONCLUSIONS

The results suggested that vanillic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6W4B enzyme of corona virus had SMILES code C[NH2+]CC(=O)c1ccc(O)c(O)c1.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	C[NH2+]CC(=O)c1ccc(O)c(O)c1	15.8795	16.340699999999998

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore Nc1ccc(Nc2ccccc2)cc1 (SMILES)

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Received: 24 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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Keywords: Corona, Virus, Docking, Pharmacophore

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	Nc1ccc(Nc2ccccc2)cc1	15	21.8445

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore [O-]C(=O)C(=O)Cc1ccccc1 (SMILES)

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Received: 25 Mar 2020 Revised: 27 Apr 2020 Accepted: 28 May 2020

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RESULTS AND DISCUSSION

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1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	[O-]C(=O)C(=O)Cc1ccccc1	25.058900000000001	31.759699999999999

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore NC(=S)Nc1ccccc1O (SMILES)

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RESEARCH ARTICLE

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1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	Oc1cc([O-])nc2ccccc12	15.93	30.358699999999999

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore COc1cc(Cl)ccc1O (SMILES)

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Received: 24 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6W4B enzyme of corona virus was identified. A pharmacophore equivalent to vanillic acid obtained from cocoa plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code COc1cc(Cl)ccc1O.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive

value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with vanillic acid of cocoa plant. The important enzyme of corona virus chosen was 6W4B.

RESULTS AND DISCUSSION

Table 1 shows that vanillic acid can block 6W4B enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6W4B. The pharmacophore had SMILES code COc1cc(Cl)ccc1O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that vanillic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6W4B enzyme of corona virus had SMILES code COc1cc(Cl)ccc1O.

REFERENCES

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	COc1cc(Cl)ccc1O	12.2112	17.491099999999999

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RESEARCH ARTICLE

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	OC(=O)C[NH2+]Cc1ccccc1	27.236599999999999	24.170200000000001

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1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	OC(=O)CCc1ncccn1	24.9344	18.7864

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore NC1=CC(=O)NC(=O)N1CC=C (SMILES)

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Keywords: Corona, Virus, Docking, Pharmacophore

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1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	NC1=CC(=O)NC(=O)N1CC=C	14.8622	21.369499999999999

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore CCNC(=S)SCCC(=O)O (SMILES)

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RESULTS AND DISCUSSION

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Table 1 shows that vanillic acid can block 6W4B enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6W4B. The pharmacophore had SMILES code CC(=O)OCCc1scnc1C. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that vanillic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6W4B enzyme of corona virus had SMILES code CC(=O)OCCc1scnc1C.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	CC(=O)OCCc1scnc1C	19.974499999999999	19.042300000000001

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore CCOC(=N)c1ccc(O)cc1 (SMILES)

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Received: 24 Mar 2020 Revised: 27 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6W4B enzyme of corona virus was identified. A pharmacophore equivalent to vanillic acid obtained from cocoa plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CCOC(=N)c1ccc(O)cc1.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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2	Pharmacophore	CCOC(=N)c1ccc(O)cc1	14.7735	16.330300000000001

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore CN1CCCN2CCCN=C12 (SMILES)

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RESULTS AND DISCUSSION

Table 1 shows that vanillic acid can block 6W4B enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6W4B. The pharmacophore had SMILES code CN1CCCN2CCCN=C12. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	CN1CCCN2CCCN=C12	14.516500000000001	17.732800000000001

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore O=C1N[C@H](CO1)c2ccccc2 (SMILES)

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Received: 23 Mar 2020 Revised: 25 Apr 2020 Accepted: 28 May 2020

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RESULTS AND DISCUSSION

Table 1 shows that vanillic acid can block 6W4B enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6W4B. The pharmacophore had SMILES code O=C1N[C@H](CO1)c2ccccc2. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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SL NO	Type	Compound	"-C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	O=C1N[C@H](CO1)c2ccccc2	19.6934	23.735199999999999

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore CC(=O)NC1=NC(=O)NC=C1 (SMILES)

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Keywords: Corona, Virus, Docking, Pharmacophore

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore CC(=O)O[C@@H]1CS[C@H](O1)C(=O)O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6W4B enzyme of corona virus was identified. A pharmacophore equivalent to vanillic acid obtained from cocoa plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(=O)O[C@@H]1CS[C@H](O1)C(=O)O.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with vanillic acid of cocoa plant. The important enzyme of corona virus chosen was 6W4B.

RESULTS AND DISCUSSION

Table 1 shows that vanillic acid can block 6W4B enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6W4B. The pharmacophore had SMILES code CC(=O)O[C@@H]1CS[C@H](O1)C(=O)O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that vanillic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6W4B enzyme of corona virus had SMILES code CC(=O)O[C@@H]1CS[C@H](O1)C(=O)O.

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2	Pharmacophore	CC(=O)O[C@@H]1CS[C@H](O1)C(=O)O	21.960599999999999	25.2029

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RESEARCH ARTICLE

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore OC(=O)c1[nH]c(C(=O)O)c2OCCOc12 (SMILES)

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore ONS(=O)(=O)c1ccccc1 (SMILES)

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore Cc1ccc(cc1)S(=O)(=O)[N-]Cl (SMILES)

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RESULTS AND DISCUSSION

Table 1 shows that vanillic acid can block 6W4B enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6W4B. The pharmacophore had SMILES code Cc1ccc(cc1)S(=O)(=O)[N-]Cl. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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Table 1 shows that vanillic acid can block 6W4B enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6W4B. The pharmacophore had SMILES code CCOC(OCC)n1ccnc1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that vanillic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6W4B enzyme of corona virus had SMILES code CCOC(OCC)n1ccnc1.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	CCOC(OCC)n1ccnc1	25.751300000000001	26.4498

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore CC1(C)O[C@@H](CC(=O)O)C(=O)O1 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6W4B enzyme of corona virus was identified. A pharmacophore equivalent to vanillic acid obtained from cocoa plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC1(C)O[C@@H](CC(=O)O)C(=O)O1.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

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Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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RESEARCH ARTICLE

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1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	N[C@@H](CS(=O)CC=C)C(=O)O	15.767300000000001	24.476900000000001

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RESEARCH ARTICLE

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	N[C@@H](CSc1nccs1)C(=O)O	16.0032	20.911999999999999

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore CN1C(=O)N=C([O-])c2c1ncn2C (SMILES)

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1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	CN1C(=O)N=C([O-])c2c1ncn2C	26.298200000000001	37.310299999999998

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RESEARCH ARTICLE

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SL NO	Type	Compound	"-C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	CC(=O)[C@@H]1C(=O)OC(=CC1=O)C	11.9079	18.036100000000001

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore CNC(=O)CN1C(=O)CCC1=O (SMILES)

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Received: 24 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6W4B enzyme of corona virus was identified. A pharmacophore equivalent to vanillic acid obtained from cocoa plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CNC(=O)CN1C(=O)CCC1=O.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with vanillic acid of cocoa plant. The important enzyme of corona virus chosen was 6W4B.

RESULTS AND DISCUSSION

Table 1 shows that vanillic acid can block 6W4B enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6W4B. The pharmacophore had SMILES code CNC(=O)CN1C(=O)CCC1=O. Positive values of "-CDOCK Energy and -CDOCK interaction energy"indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that vanillic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6W4B enzyme of corona virus had SMILES code CNC(=O)CN1C(=O)CCC1=O.

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2	Pharmacophore	CNC(=O)CN1C(=O)CCC1=O	26.658000000000001	26.259599999999999

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RESEARCH ARTICLE

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by Pharmacophore O=C1NC(=O)C2=NC=CNC2=N1 (SMILES)

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	vanillic acid	11.7323	23.155000000000001
2	Pharmacophore	O=C1NC(=O)C2=NC=CNC2=N1	13.394500000000001	18.870100000000001

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore Clc1nc(Cl)nc(n1)N2CCCc3ccccc23 (SMILES)

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Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

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Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code Clc1nc(Cl)nc(n1)N2CCCc3ccccc23. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	Clc1nc(Cl)nc(n1)N2CCCc3ccccc23	34.840499999999999	28.66

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Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CC(=O)c1cc2CCCCc2c(O)c1O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	CC(=O)c1cc2CCCCc2c(O)c1O	24.312799999999999	28.4055

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RESEARCH ARTICLE

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Keywords: Corona, Virus, Docking, Pharmacophore

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RESEARCH ARTICLE

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2	Pharmacophore	COC(=O)CS[C@H](C)CC(=O)OC	25.516500000000001	25.673100000000002

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The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code CCC(=O)Oc1sc(NCCc2ccccc2)[n+](C)c1C.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CCC(=O)Oc1sc(NCCc2ccccc2)[n+](C)c1C	35.848300000000002	39.304099999999998

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CCc1c(C(=O)OC)c2cc(O)ccc2n1Cc3ccccc3 (SMILES)

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Received: 25 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CCc1c(C(=O)OC)c2cc(O)ccc2n1Cc3ccccc3.

Keywords: Corona, Virus, Docking, Pharmacophore

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RESULTS AND DISCUSSION

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CCOC(=O)Cc1c(C)[nH]c2ccc(cc12)C(C)C (SMILES)

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore O=C1CCCCCN1SSN2CCCCCC2=O (SMILES)

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Received: 23 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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2	Pharmacophore	O=C1CCCCCN1SSN2CCCCCC2=O	25.1401	35.978299999999997

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore C[C@H](SCS[C@H](C)C(=O)O)C(=O)O (SMILES)

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RESEARCH ARTICLE

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CC(C)c1cc(SC#N)c(C)cc1O	22.133700000000001	24.347200000000001

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CCOC(=O)C(N(C)C)C(=O)OCC (SMILES)

S. Swain

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Received: 23 Mar 2020 Revised: 25 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CCOC(=O)C(N(C)C)C(=O)OCC.

Keywords: Corona, Virus, Docking, Pharmacophore

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"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

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used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with caffeic acid of coffee plant. The important enzyme of corona virus chosen was 6Y84.

RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CCOC(=O)C(N(C)C)C(=O)OCC. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code CCOC(=O)C(N(C)C)C(=O)OCC.

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RESEARCH ARTICLE

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1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	Cc1cc(C)c(CC(=O)O)c(C)c1	23.6599	23.025400000000001

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore OC(=O)[C@@H]1CS[C@@H](N1)c2ccc(cc2)[C@@H]3N[C@@H](CS3)C(=O)O (SMILES)

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(C)(C)\C(=C\C(=O)C(C)(C)C)\[O-] (SMILES)

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"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code C[NH2+]CC(=O)c1ccc(O)c(O)c1.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the

viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with caffeic acid of coffee plant. The important enzyme of corona virus chosen was 6Y84.

RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code C[NH2+]CC(=O)c1ccc(O)c(O)c1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code C[NH2+]CC(=O)c1ccc(O)c(O)c1.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	C[NH2+]CC(=O)c1ccc(O)c(O)c1	41.732900000000001	42.0627

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CCOC(=O)[C@H]1CC[N@@H+](Cc2ccccc2)CC1=O (SMILES)

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Received: 25 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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Received: 24 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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RESEARCH ARTICLE

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Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code C[NH+]1CCN(Cc2ccccc2)CC1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code C[NH+]1CCN(Cc2ccccc2)CC1.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	C[NH+]1CCN(Cc2ccccc2)CC1	22.683	36.274099999999997

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(C)[C@@H]1CC[C@@H](C)C[C@H]1OC(=O)C(O)O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(C)[C@@H]1CC[C@@H](C)C[C@H]1OC(=O)C(O)O.

Keywords: Corona, Virus, Docking, Pharmacophore

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"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

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Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

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2	Pharmacophore	CN(C)CCN(Cc1ccccc1)c2ccccn2	27.035399999999999	33.035400000000003

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(=O)Nc1ccc(cc1)S(=O)(=O)NC2(CCCCC2)C(=O)O (SMILES)

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore OC(=O)CCc1ncccn1 (SMILES)

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	Cc1oc(C[N+](C)(C)C)cc1	23.050999999999998	26.188600000000001

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CN(C)CCS[C@H](CO)c1ccccc1 (SMILES)

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Received: 25 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CN(C)CCS[C@H](CO)c1ccccc1.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

Methodology: "Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu

used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with caffeic acid of coffee plant. The important enzyme of corona virus chosen was 6Y84.

RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CN(C)CCS[C@H](CO)c1ccccc1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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2	Pharmacophore	CCNC(=S)SCCC(=O)O	20.849499999999999	22.495899999999999

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2	Pharmacophore	CC(C)COC(=O)OCC(C)C	29.642099999999999	24.799099999999999

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RESEARCH ARTICLE

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"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used

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RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code COC(=O)[C@](C)(N)Cc1ccc(O)cc1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code COC(=O)[C@](C)(N)Cc1ccc(O)cc1.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	COC(=O)[C@](C)(N)Cc1ccc(O)cc1	28.4617	27.9192

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(C)C(=O)OC[C@H](C)c1ccccc1 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(C)C(=O)OC[C@H](C)c1ccccc1.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

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2	Pharmacophore	CC(C)C(=O)OC[C@H](C)c1ccccc1	25.1935	24.3704

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore OC(=O)CCCc1ccc(cc1)C(=O)c2ccccc2C(=O)O (SMILES)

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1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	OC(=O)CCCc1ccc(cc1)C(=O)c2ccccc2C(=O)O	26.872499999999999	33.190399999999997

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CCOC(=O)[C@](C)(OC(=O)C)C(=O)C (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CCOC(=O)[C@](C)(OC(=O)C)C(=O)C.

Keywords: Corona, Virus, Docking, Pharmacophore

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1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CCOC(=O)[C@](C)(OC(=O)C)C(=O)C	26.6343	25.241399999999999

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(=O)OCCc1scnc1C (SMILES)

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1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CC(=O)OCCc1scnc1C	23.5275	21.299299999999999

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RESEARCH ARTICLE

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Sujata Acharya

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Received: 24 Mar 2020 Revised: 25 Apr 2020 Accepted: 28 May 2020

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore O=C1N[C@H](CO1)c2ccccc2 (SMILES)

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	O=C1N[C@H](CO1)c2ccccc2	24.3538	28.484400000000001

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(=O)NC1=NC(=O)NC=C1 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(=O)NC1=NC(=O)NC=C1.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used

CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with caffeic acid of coffee plant. The important enzyme of corona virus chosen was 6Y84.

RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CC(=O)NC1=NC(=O)NC=C1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code CC(=O)NC1=NC(=O)NC=C1.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CC(=O)NC1=NC(=O)NC=C1	21.789300000000001	25.02

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CN(C)Cc1oc(CO)cc1 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CN(C)Cc1oc(CO)cc1.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CN(C)Cc1oc(CO)cc1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code CN(C)Cc1oc(CO)cc1.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CN(C)Cc1oc(CO)cc1	20.805	21.0305

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(=O)O[C@@H]1CS[C@H](O1)C(=O)O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(=O)O[C@@H]1CS[C@H](O1)C(=O)O.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value

of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with caffeic acid of coffee plant. The important enzyme of corona virus chosen was 6Y84.

RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CC(=O)O[C@@H]1CS[C@H](O1)C(=O)O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code CC(=O)O[C@@H]1CS[C@H](O1)C(=O)O.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CC(=O)O[C@@H]1CS[C@H](O1)C(=O)O	23.922999999999998	26.265599999999999

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore NS(=O)(=O)c1cc(C(=O)O)c(NCc2ccccc2)cc1Cl (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code NS(=O)(=O)c1cc(C(=O)O)c(NCc2ccccc2)cc1Cl.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used

CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with caffeic acid of coffee plant. The important enzyme of corona virus chosen was 6Y84.

RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code NS(=O)(=O)c1cc(C(=O)O)c(NCc2ccccc2)cc1Cl. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	NS(=O)(=O)c1cc(C(=O)O)c(NCc2ccccc2)cc1Cl	32.0548	39.004199999999997

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore COc1cc2C[NH2+][C@@H](Cc2cc1OC)C(=O)O (SMILES)

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ABSTRACT

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Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

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METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used

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RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code COc1cc2C[NH2+][C@@H](Cc2cc1OC)C(=O)O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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2	Pharmacophore	COc1cc2C[NH2+][C@@H](Cc2cc1OC)C(=O)O	26.542999999999999	38.680300000000003

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(=O)CCc1c(C)c(OC(=O)C)c(C)c(C)c1OC(=O)C (SMILES)

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CC(=O)CCc1c(C)c(OC(=O)C)c(C)c(C)c1 OC(=O)C	38.690399999999997	36.101799999999997

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(C)C1=CC(=O)Oc2c3CCCN4CCCc(cc12)c34 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(C)C1=CC(=O)Oc2c3CCCN4CCCc(cc12)c34.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used

CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with caffeic acid of coffee plant. The important enzyme of corona virus chosen was 6Y84.

RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CC(C)C1=CC(=O)Oc2c3CCCN4CCCc(cc12)c34. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code CC(C)C1=CC(=O)Oc2c3CCCN4CCCc(cc12)c34.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CC(C)C1=CC(=O)Oc2c3CCCN4CCCc(cc12)c34	20.3233	34.435400000000001

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore OC(=O)c1[nH]c(C(=O)O)c2OCCOc12 (SMILES)

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ABSTRACT

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore OC[C@@H](O)COc1ccc(Cc2ccc(OC[C@H](O)CO)cc2)cc1 (SMILES)

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ABSTRACT

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(=O)C1=C([O-])C=C(C)OC1=O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(=O)C1=C([O-])C=C(C)OC1=O.

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CCOC(OCC)n1ccnc1 (SMILES)

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ABSTRACT

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RESEARCH ARTICLE

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Namita Panda

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore OC[C@H](Cc1cccc(O)c1)[C@H](CO)Cc2cccc(O)c2 (SMILES)

M. K. Sahu

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RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code OC[C@H](Cc1cccc(O)c1)[C@H](CO)Cc2cccc(O)c2. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code OC[C@H](Cc1cccc(O)c1)[C@H](CO)Cc2cccc(O)c2.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	OC[C@H](Cc1cccc(O)c1)[C@H](CO) Cc2cccc(O)c2	27.309100000000001	37.940300000000001

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(C)[C@H]1CC[C@H](C)C[C@@H]1OCC(=O)O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(C)[C@H]1CC[C@H](C)C[C@@H]1OCC(=O)O.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized.
Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used

CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with caffeic acid of coffee plant. The important enzyme of corona virus chosen was 6Y84.

.RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CC(C)[C@H]1CC[C@H](C)C[C@@H]1OCC(=O)O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CC(C)[C@H]1CC[C@H](C)C[C@@H]1OCC(=O)O	22.3278	32.431199999999997

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CCN1C=C(C(=O)[O-])C(=O)c2ccc(C)nc12 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CCN1C=C(C(=O)[O-])C(=O)c2ccc(C)nc12.

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Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CCN1C=C(C(=O)[O-])C(=O)c2ccc(C)nc12. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CCN1C=C(C(=O)[O-])C(=O)c2ccc(C)nc12	27.188500000000001	33.513100000000001

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(C)CNC(=O)N1CCNC1=O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(C)CNC(=O)N1CCNC1=O.

Keywords: Corona, Virus, Docking, Pharmacophore

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CC(C)CNC(=O)N1CCNC1=O	22.113	26.7883

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CCC(=C1C(=O)CC(CC1=O)C(=O)[O-])[O-] (SMILES)

Manju Palei

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CCC(=C1C(=O)CC(CC1=O)C(=O)[O-])[O-].

Keywords: Corona, Virus, Docking, Pharmacophore

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RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CCC(=C1C(=O)CC(CC1=O)C(=O)[O-])[O-]. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CCC(=C1C(=O)CC(CC1=O)C(=O)[O-])[O-]	29.511099999999999	36.280700000000003

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore COC(=O)CCC1=NNC(=O)NC1=O (SMILES)

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ABSTRACT

Abstract

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code COC(=O)CCC1=NNC(=O)NC1=O.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

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METHODOLOGY

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RESULTS AND DISCUSSION

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1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	COC(=O)CCC1=NNC(=O)NC1=O	22.966799999999999	23.5306

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(C)OC(=O)[C@H](C)NC1=NNC(=S)NC1=O (SMILES)

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CC(C)OC(=O)[C@H](C)NC1=NNC(=S)NC1=O	27.760000000000002	30.485700000000001

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RESEARCH ARTICLE

Deactivation of 6Y84 ENzyme of Corona by Pharmacophore CC(C)CCOC(=O)[C@H](C)SC1=NNC(=O)NC1=O (SMILES)

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Received: 24 Mar 2020 Revised: 27 Apr 2020 Accepted: 28 May 2020

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ABSTRACT

Abstract

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(C)CCOC(=O)[C@H](C)SC1=NNC(=O)NC1=O.

Keywords: Corona, Virus, Docking, Pharmacophore

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"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral

enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with caffeic acid of coffee plant. The important enzyme of corona virus chosen was 6Y84.

RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CC(C)CCOC(=O)[C@H](C)SC1=NNC(=O)NC1=O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code CC(C)CCOC(=O)[C@H](C)SC1=NNC(=O)NC1=O.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	CC(C)CCOC(=O)[C@H](C)SC1=NNC(=O)NC1=O	25.953700000000001	31.289200000000001

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CN1C(=O)N(C)c2ncn(Cc3ncc[nH]3)c2C1=O (SMILES)

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore COC(=O)CCC1=NO[C@H](C[C@@H]2CC(=NO2)CCC(=O)OC)C1 (SMILES)

Satyabrata Palei

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code COC(=O)CCC1=NO[C@H](C[C@@H]2CC(=NO2)CCC(=O)OC)C1.

Keywords: Corona, Virus, Docking, Pharmacophore

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RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code COC(=O)CCC1=NO[C@H](C[C@@H]2CC(=NO2)CCC(=O)OC)C1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CCOC(=O)CCc1ccc(\C=C\C(=O)OCC)[nH]1 (SMILES)

S. Naik

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ABSTRACT

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore Cc1c(CO)sc[n+]1Cc2ccccc2 (SMILES)

Monalisa Joshi

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Received: 24 Mar 2020 Revised: 26 Apr 2020 Accepted: 28 May 2020

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RESEARCH ARTICLE

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Lokanath Meher

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(=O)\C=C\c1cc(C)[nH]c1C (SMILES)

Ramesh Sahu

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(=O)\C=C\c1cc(C)[nH]c1C.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used

CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with caffeic acid of coffee plant. The important enzyme of corona virus chosen was 6Y84.

RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CC(=O)\C=C\c1cc(C)[nH]c1C. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code CC(=O)\C=C\c1cc(C)[nH]c1C.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CC(=O)\C=C\c1cc(C)[nH]c1C	22.8323	23.602699999999999

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CN(C)Cc1c(C)[nH]c(C)c1CN(C)C (SMILES)

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2	Pharmacophore	CN(C)Cc1c(C)[nH]c(C)c1CN(C)C	28.175000000000001	26.5535

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CNC(=O)CN1C(=O)CCC1=O (SMILES)

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ABSTRACT

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Keywords: Corona, Virus, Docking, Pharmacophore

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Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CNC(=O)CN1C(=O)CCC1=O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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2	Pharmacophore	CNC(=O)CN1C(=O)CCC1=O	24.157699999999998	23.677600000000002

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore NC(=O)c1ccc(NCC(=O)O)cc1 (SMILES)

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ABSTRACT

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Keywords: Corona, Virus, Docking, Pharmacophore

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RESULTS AND DISCUSSION

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1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	NC(=O)c1ccc(NCC(=O)O)cc1	26.2881	27.9223

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(C)c1cc(OC(=O)C)c(C)cc1OCCN(C)C (SMILES)

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ABSTRACT

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RESEARCH ARTICLE

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enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with caffeic acid of coffee plant. The important enzyme of corona virus chosen was 6Y84.

RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code C[C@H](C(=O)C)n1c(CN2CCOCC2)nc3N(C)C(=O)N(C)C(=O)c13. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

CONCLUSIONS

The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code C[C@H](C(=O)C)n1c(CN2CCOCC2)nc3N(C)C(=O)N(C)C(=O)c13.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	C[C@H](C(=O)C)n1c(CN2CCOCC2) nc3N(C)C(=O)N(C)C(=O)c13	25.3232	39.783700000000003

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CN1C(=O)NC(=O)c2[nH]c(nc12)N3CCN(CCO)CC3 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CN1C(=O)NC(=O)c2[nH]c(nc12)N3CCN(CCO)CC3.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used

CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with caffeic acid of coffee plant. The important enzyme of corona virus chosen was 6Y84.

RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CN1C(=O)NC(=O)c2[nH]c(nc12)N3CCN(CCO)CC3. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code CN1C(=O)NC(=O)c2[nH]c(nc12)N3CCN(CCO)CC3.

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1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CN1C(=O)NC(=O)c2[nH]c(nc12)N3CCN(CCO)CC3	23.436199999999999	38.328400000000002

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CCOC(=O)CN1C(=O)C=Nc2ccccc12 (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CCOC(=O)CN1C(=O)C=Nc2ccccc12.

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Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CCOC(=O)CN1C(=O)C=Nc2ccccc12. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CCOC(=O)CN1C(=O)C=Nc2ccccc12	28.611000000000001	32.424100000000003

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(C)(C)c1cc(Cn2cc[nH+]c2)ccc1O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(C)(C)c1cc(Cn2cc[nH+]c2)ccc1O.

Keywords: Corona, Virus, Docking, Pharmacophore

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MATERIALS AND METHODS

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RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CC(C)(C)c1cc(Cn2cc[nH+]c2)ccc1O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CC(C)(C)c1cc(Cn2cc[nH+]c2)ccc1O	31.2364	37.330800000000004

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(C)(Oc1ccc(Cl)cc1)C(=O)OCC(=O)NCC(=O)O (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code CC(C)(Oc1ccc(Cl)cc1)C(=O)OCC(=O)NCC(=O)O.

Keywords: Corona, Virus, Docking, Pharmacophore

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MATERIALS AND METHODS

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value

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RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CC(C)(Oc1ccc(Cl)cc1)C(=O)OCC(=O)NCC(=O)O. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CC(C)(Oc1ccc(Cl)cc1)C(=O)OCC(=O)NCC(=O)O	36.346800000000002	38.7971

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore Nc1c(Br)cc(Br)cc1CN[C@@H]2CC[C@@H](O)CC2 (SMILES)

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore NCCC(=O)NCCc1ncc[nH]1 (SMILES)

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CONCLUSIONS

The results suggested that caffeic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound which may deactivate 6Y84 enzyme of corona virus had SMILES code NCCC(=O)NCCc1ncc[nH]1.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	NCCC(=O)NCCc1ncc[nH]1	31.153300000000002	29.431999999999999

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore C[C@H](C[N+](C)(C)C)OC(=O)N (SMILES)

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ABSTRACT

"Corona virus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome" and presently, killed many people worldwide. Researchers are still struggling to find a cure. Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that may deactivate 6Y84 enzyme of corona virus was identified. A pharmacophore equivalent to caffeic acid obtained from coffee plant was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was a compound with SMILES code C[C@H](C[N+](C)(C)C)OC(=O)N.

Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

MATERIALS AND METHODS

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a phytochemical that can deactivate the viral enzyme. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used

CHARMm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value of both the parameters indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with caffeic acid of coffee plant. The important enzyme of corona virus chosen was 6Y84.

RESULTS AND DISCUSSION

Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code C[C@H](C[N+](C)(C)C)OC(=O)N. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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Table 1. Results of CDOCK

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	C[C@H](C[N+](C)(C)C)OC(=O)N	24.539300000000001	26.479299999999999

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RESEARCH ARTICLE

Deactivation of 6Y84 Enzyme of Corona by Pharmacophore CC(C)(C)NC[C@H](O)c1cc(Cl)c(N)c(Cl)c1 (SMILES)

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ABSTRACT

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Keywords: Corona, Virus, Docking, Pharmacophore

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has caused the death of many people all over the world. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that still the researchers are struggling to discover a drug that can prevent corona. [2]. Countries are trying to fight through lockdown. However, that strategy has hit the economy badly. Thus, there is a significant need to develop a treatment for corona. The mankind is doing extensive research to fight back the deadly virus. The goal of the present work is to identify a pharmacophore against corona through *in silico* analysis.

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Table 1 shows that caffeic acid can block 6Y84 enzyme of corona virus. A pharmacophore was identified which may cure the disease by blocking the enzyme 6Y84. The pharmacophore had SMILES code CC(C)(C)NC[C@H](O)c1cc(Cl)c(N)c(Cl)c1. Positive values of "-CDOCK Energy and -CDOCK interaction energy" indicated that the pharmacophore may fight against corona virus. Further wet lab test is required to prove it. However, such analysis may reduce the number of trials. The qualitative and quantitative strengths of interactions between ligands and an enzyme is essential in drug discovery. Reliable estimation of binding interaction may improve the ligand selection. Molecular docking is usually compared to a Lock and Key process. The conformation of the ligand and enzyme does not change during binding. Ligands are often flexible and occupy multiple conformations in solution. CDOCK method considers the multiple conformations and the influence on the interaction. The result shown corresponds to the conformation that resulted in the highest value of - C DOCKER ENERGY.

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1	Phytochemical	caffeic acid	26.933700000000002	27.4209
2	Pharmacophore	CC(C)(C)NC[C@H](O)c1cc(Cl)c(N)c(Cl)c1	22.214600000000001	27.938600000000001

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RESEARCH ARTICLE

Study of Aerodynamics of a Vehicle and its Stability

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ABSTRACT

This article deals with the study on the effects of aerodynamic modelling of vehicle.The investigation was carried out for the pressure, velocity, and vorticity distribution around the vehicle environment. This modelling is based upon the meshless simulation techniques and its application to find a quick and more accurate simulation for the scenario. The computational techniques should not be time taking; if it will be so, then it increases the cost of simulation. The attempt made here is to just give some idea of meshless simulation techniques for external flow over bodies.

Keywords: CFD simulation, aerodynamic body, air flow around car, techniques to solve CFD, meshless simulation.

INTRODUCTION

In today's word, we are focused of getting high speed vehicles with reduced drag forces and vortices acting on it. The drag forces reduce the capability of stability of vehicles under high speed conditions. Also, it is very essential to reduce the lift acting on the high-speed cars by proving additional surface features like spoilers.Malizia et al. investigated the CFD simulation of spoked wheel cycle [1]. Blocken et al. studied the consequences of force-drag influenced by the car due to the cycle by CFD [2]. Deckers et al. investigated the effects of fire incar parking by full scale CFD simulations [3].Fintelman et al. observed the influence of flow around the cyclist due to cross winds [4].Thabet et al. investigated the CFD simulation of a flow around the car [5].The solution setup of the 3d fluid flow surrounding the environment of a reference vehicleand the observation of the effects of forces created by the air flow on the vehicle surface. This is a typical external aerodynamic case using the virtual wind tunnel.

This case study shows how to:

- Importingthe geometry from CAD importer.

- Checking the model imported to the system.
- Virtual wind tunnel Explorer is used for the working with the log file.
- Flow variables is observed on the vehicle total surfaces.

METHODOLOGY

Geometrical modelling and steps

The modelling can be done on a variety of commercial software available in market. Then, the modelling is imported to the commercial software.
Main menu > Geometry > Import a new geometry. The Model Units window, shown in the figure below, will appear automatically.Imported geometry will be shown in the Graphic View, and it will appear as a Shape in the Geometricalcategoryin Project sub-Tree.

Model checking

(a) Orientation of the provided vehicle in the Graphical View window is checked. Here, the height is represented by the Y direction; the direction of flow is from -X to +X.
(b) Information related to the geometry can be showed by only clicking on it, right clicking on the Graphic View window and choosing in the Graphic View Menu > Show geometrical properties
(c) Dimensions of the vehicle is measured. Main Menu is pressed by selecting the geometry.>

Geometry > Dimensions or
Length is in X direction.
Height is in Y direction.
Width is in Z direction.

Keep the geometry selected and click again to hide the dimensions.
(d) Surface tessellation quality is checked. To this end: the geometry of the object is selected, then right clicked on the Graphical View window and choose Graphic View Menu > Visualization mode > Mesh

(e) Check the surface normal enabling the culling; thus, selecting the geometrical object, then right clicking on the Graphical View window and choosing Graphical View of the Menu > Back-faced culling is selected. Graphic View Menu > Reverse orientation. Eventually, leaving the normal pointing towards the exterior of the car as shown in the figure below on the right.

If the model has holes, fluid will leak inside. This fluid inside the geometry is initialised with the inlet velocity condition as the rest of the fluid but, because it is confined, generates pressure waves inside of the geometry that lead to wrong forces. Furthermore, closed volumes with a small opening will equilibrate the interior pressure to the local static pressure at the hole, leading to wrong overall forces.

Problem setup

Engine settings Project Tree > Environment > Engine:

(a) Turbulence settings > Turbulence model: Automatic
(b) Turbulence settings > Turbulence generation: Off
(c) Leave the default Advanced Options.

Environment settings Project Tree > Environment > Environment:

(a) Global attributes > Domain type: Virtual wind tunnel
(b) Global attributes > Ext. acceleration laws: leave it to zero
(c) Global attributes > Initial conditions: Wind tunnel default

When using the Wind tunnel default initial condition, software initializes the velocity field according to the inlet Velocity laws. This is a good practice for external aerodynamic simulations.
(d) Keep Reference area as Front and Reference velocity as Automatic,
(e) Wind tunnel > Lateral boundaries: Periodic. Symmetric lateral boundaries could be useful to simulate half vehicle
(f) Wind tunnel > Boundary condition: Velocity. Set a Velocity law at inlet equal to (50, 0, 0) m/s
Material settings:
Keep the default parameters of air in Project Tree > Materials.
Geometry settings:
Project Tree > Geometry > Shape-Asmo

Simulation settings

Project Tree > Simulation:
(a) Simulation time: 0.15 seconds
(b) Timing mode: Automatic in fixed.
(c) Timing step mode >Courant number: 1
(d) Resolution > Resolved scale: 0.2 metres (resolution at the far field)
(e) Resolution > Refinement algorithm: Adapt to walls and dynamically adapt to wake
(f) Resolution > Wake resolution: 0.0125 metres
(g) Resolution > Wake refinement threshold: Automatic
(h) Resolution > Shapes refinement > Shape- asmo >Target resolved scale: This represent the near wall resolution, set it equal to Wake resolution and leave Curvature adapted Off.
(i) Resolution > Regions > Refinement transition length: 3

Due to the Cartesian structure of the lattice, the choice of the different resolutions must be related by a factor 2 n, with n an integer. In this tutorial, n=4: h = 0.2/2 4 = 0.0125 m near the wall. The wake is developing only because of the flow surrounding a body; therefore, the wake resolution must be equal or greater than the near wall resolution.

(i) Store data in the Folder "asmo", with a Frames frequency of 200 Hz and Numerical data frequency to Frames frequency; this will save hard disk space although the curves in the Function Viewer will have less points than if Solver time step frequency had been chosen.

(g) Leave disabled the computation of averaged fields and markers, as long as resume file

RESULTS AND DISCUSSION

Cutting plane is created. Go to the Project Tree > Post Processing tab and:
(a) Right-click on Cutting planes > Add cutting plane or press in the Post-Processing Toolbar (b) Visualise the velocity in the cutting plane by setting: Cutting plane > Visualisation mode: 3d field, and choose the Field: Velocity
(c) Activate the interpolation mode: General > Interpolation mode: Convolution

(d) Set the velocity range to [0,60]: Main menu > Simulation data > Analysis settings or press in Toolbar Data Processing.
(e) Select the right view
(f) Press Play Note that the internal domain is initialized (frame 0) with the inlet velocity of the virtual wind tunnel.

Fig. 1 shows the velocity contour of flow around the vehicle, it can be inferred that the velocity at the front edge is low and should be eliminated. This is because of present of flat area portion near the front edge of the vehicle. Also, the velocity at the top of the vehicle is high and hence it is aerodynamically good surface.

Fig. 2 shows the pressure contour of the environment around the vehicle, and it clearly states that the pressure is high enough to create drag at high speed conditions. The pressure at the rear end is low, and hence the vehicle is not aerodynamically suitable to be operated at prescribed conditions.

The Fig. 3 shows the vorticity distribution around the environment, it clearly depicts the creation of vorticity around the frontal and rear ends of the vehicle. Therefore, it creates instability of the vehicle; and it seriously needs modification.

The Fig. 4 shows the turbulence intensity distribution around the environment of the vehicle, it clearly shows the turbulence intensity is maximum at the rear end. Therefore, the design should be considered as it may not create so much of turbulence in the front end.

CONCLUSION

The process of creation of CFD flow around the vehicle is defined;also, selection of an aerodynamic surface upon the vehicle is observed. The vehicle is to be modified on the basis of aerodynamic flow around it. There should be low turbulence in order to go for the stability of the vehicle.

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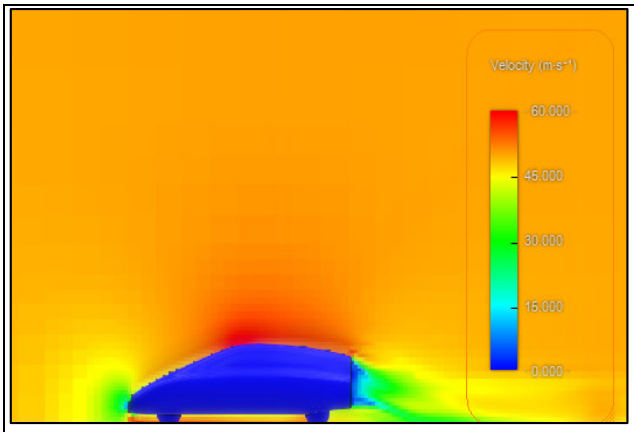

Fig.1. Velocity distribution around the environment

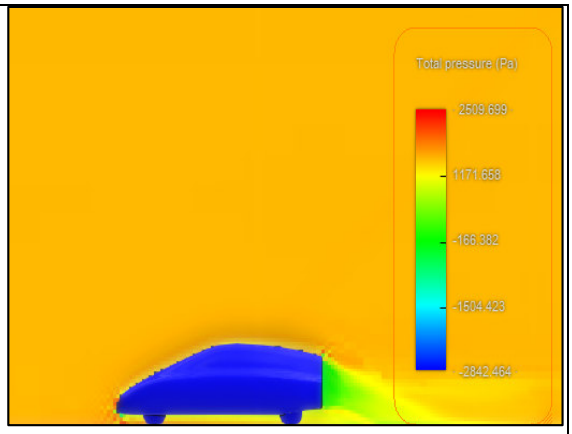

Fig.2.Pressure distribution around the environment

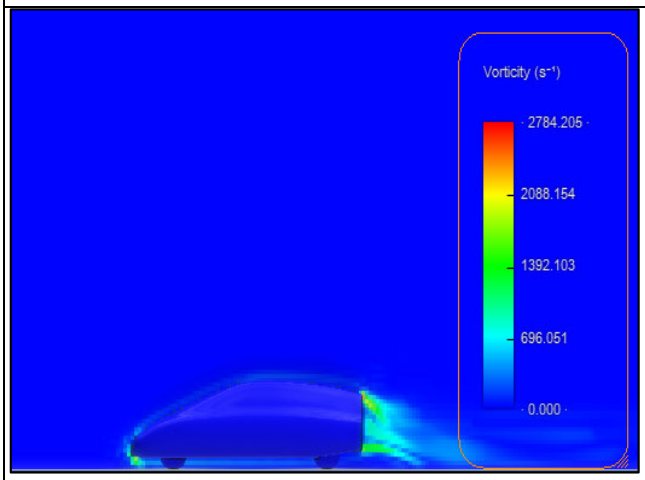

Fig. 3. Vorticity distribution around the environment

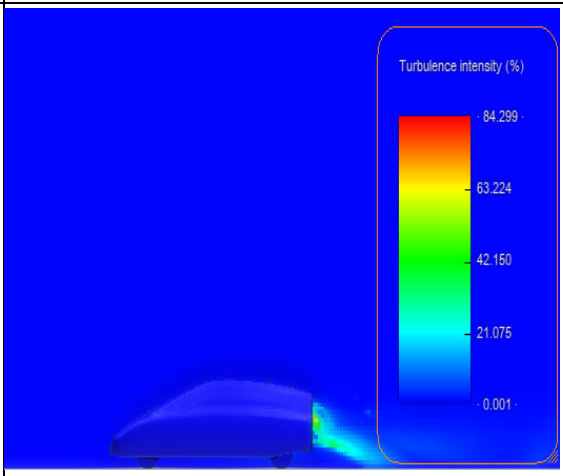

Fig.4.Turbulence intensity distribution around the environment

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RESEARCH ARTICLE

Experimental Analysis of a V-Shaped Double Rectangular Tube Parabolic Trough Collector

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ABSTRACT

The influence of various parameters such as concentration ratio and $\eta_{thermal}$ was analysed on the performance of solar trough collector in this experimental work. This paper gives a critical technological study on various types of solar thermal system. To produce electricity, Concentrated Solar Power (CSP) technologies are used widely. Among the most proven and advanced of the various CSP technologies, PTC is economically viable. To upgrade of the design and performances, modelling of these devices is an essential factor. The approach used for the thermal modelling of a PTC is to look at the realistic non-uniform solar heat flux in the azimuthal direction is introduced.

Keywords: Parabolic Trough Collector, Performance Analysis, Heat Transfer Fluid.

INTRODUCTION

The sun is at extremely at high pressure and temperature. Sun is indeed the source of all energy that we exploit for satisfying all our energy needs for wellbeing and for comfort lifestyle. Solar radiant energy is controlled using a range of recent technologies. Few examples are, solar thermal energy solar heating, photovoltaic, solar architecture, molten salt power plants and artificial photosynthesis.Every day the sun radiates large amount of energy. Utilization of solar energy is a favourable choice to find solutions to problems in the energy domain e.g.; fossil fuel exhaustion [1], global warming [2] the rising electricity consumption [3]. Solar energy has been shown to have potential to fulfil a considerable portion of the world's energy need [4]. 1.7×10^{14} kW of energy received from sun by the earth surface. 900 EJ was produced from 84 min of solar radiation. The world's energy consumption for the year 2009 is equivalent to this energy[5].

Solar collector utilises sun's irradiation and converts it to heat energy. Heat energy is converted to thermal energy with help of working fluid. As well as in domestic settings, a large number of these collectors can be combined in an array and used to generate electricity in solar thermal power plants. A solar thermal collector collects heat by absorbing sunlight [6].Solar collector is a device for power generating installations such as solar parabolic trough collector and solar towers.
According to geometrical shapes, classification of solar collectors is:-

(a) PTC (b) FPC (c) CPC

PTC Thermal analysis reveals its design criteria and heat transfer enhancement technologies. PTC consists of a parabolic reflector plate, working fluid chamber and a concentric transparent cover. [6] The transparent cover prohibits losses due to wind and the receiver tube losses from oxidation. The receiver tube is the very important component of parabolic solar panel technology. This receiver tube is embraced of an inner steel tube with discerning coating surrounded by an anti-reflective evacuated glass tube [7]. Conventional glass-to-metal seals and metal bellows are used in HCE to confirm vacuum in annular zone and assist for thermal expansion difference between the steel and glass tubes [8].The flat-plate solar collectors are and most studied technology for solar-powered domestic hot water systems. The sun heats a dark flat surface, which collects as much energy as possible, and then the energy is transferred to water, air or other fluid for further use. Black surface is absorbent of the incident solar energy. Glazing cover is a transparent layer that disseminates radiation to the absorber. It also prohibits radiative and convective heat loss from the surface. Tubes contain heating fluid to transfer the heat from the collector. Insulation covering are incorporated in sides and bottom of the collector to minimise heat losses.CPC is a concentrating collector where incident solar radiations, after reflection from the reflector, are not concentrated at a point or line [9]. It collects and focuses a larger area of sunlight onto a smaller area with minimum loss. This type of collector consists of 3 basic components: (i) receiver, (ii) cover band (iii) reflector.The receiver should have good absorbing capacity for solar radiation and should have high conductivity metals in order to conduct efficiently the absorbed heat into the heat transfer fluid [10].

METHODOLOGY

Experimental setup

The aluminium blocks are fixed in **V** shape in specified angle as shown in Fig.1. We need four similar rectangular blocks and each block is connected with each other in proper cycling process through water pipe. First, we have to take a thermos-cool sheet and cut it in round shape. The cutting sheet diameter should be same as the inner diameter of glass tube, because it has to be inserted into the glass tube.

Glass tube: The convective heat loss can be minimized by maintaining vacuum between them. The absorbed placed inside the glass tube. This tube is 60 cm length and 90 mm diameter.
Glass cover: Glue was used to fix the glass cover, half length of structure. And another half was fixed with screw. The length and breadth of glass frame were 90 cm and 60 cm respectively. The glass was fitted into the frame to make it a closed box structure. This frame is placed on the parabolic box as shown in Fig.2.

Fabrication process

Plywood, glass (flat & tube), steel sheet, iron angle, thermos-cool sheet from hardware store as per required quantity were purchased from the market. Then the plywood was cut in the workshop to a parabolic, keeping same measurement in both sides. Then the steel sheet placed between two plywood from bottom side maintains the same curve as in plywood. After completing this, the setup is required to be mounted on a stand. The stand was made

fixable by welding from iron angel. The panel and stand is mounted by not and bolt and the panel is moved towards the maximum sun intensity. This can be moved from 0-70^0 angle as per requirement. The thermos-cool sheets are cut same as glass tube inner diameter. Those sheets hold the rectangular receiver blocks in proper angle. The whole body of the panel which are made up with plywood is coated with aluminium sheet for getting the more result. This sheet is pasted by glue.

Support structure of PTC

This structure is made by 6 mm thick MS angles. The cutting was done with the help of electric iron cutter. The structure was put into a shape with the help of hammer and die. Further, they were welded together according to the design. Then the structure was fitted in the supporting structure with the help of 8 mm hexagonal type nut bolt. The mirror coated stainless steel sheet was fitted in the parabolic trough structure with help of 3 mm nut bolts. A 0.8 mm iron sheet was cut to cover both the edges of the parabolic trough structure. This sheet was attached to the parabolic trough edges. A hygrometer is used to measure the humidity and water vapour in atmosphere and soil. It is used for atmospheric temperature.

Experimental Design (Fig.3)

The experiments were carried out by adopting the following steps:

- Two parabolic shapes are created from the plywood of focal point 30 cm.
- A structure is created using two parabolic shaped plywood to hold the glass tube on a stand.
- Aluminium sheet is placed inside the structure to work as a reflector.
- Four aluminium blocks are connected internally with each other for flowing of liquid.
- Aluminium blocks are set in many angles with each other at 80, 100, 120, 140, 160, 180 degree.
- All the above equipment are taken and made a complete setup to do the experiment.
- The complete setup is placed on the roof facing towards sun for the readings.
- The various angles are set for the aluminium blocks and put inside the glass tube.
- A water pump is placed inside a bucket full of water to work as an input of our setup and then connect it with aluminium blocks through a pipe. Then we placed the outlet with other side of the glass tube and the four aluminium blocks are interconnected.
- Various readings are taken for inlet, outlet, receiver, reflector, glass tube, upper glass, ambient temperature, velocity of the air, solar radiation and humidity.
- For measuring the temperature of inlet, outlet, reflector, receiver and glass tube temperature sensor is used.

RESULTS AND DISCUSSION

From Fig.4 and 5 it can be observed that temperature at outlet, receiver block temperature and glass temperature for 120^0, 140^0 and 160^0 are in order of decreasing. This happens only due the fact that this parabolic collector has a rim angle of 120^0, so the concentrator collects and reflects the radiation in the same angle.HTF temperature & heat losses: It can be seen from Figs.6 and 7 that the outlet temperature of HTF starts increasing before 6.00 AM with glass cover case. But the temperature of HTF increases after 6.00 AM without glass cover case. Also, the HTF temperature of without glass cover ends before time as compared to with glass cover. This happens only due to fact that the convection and radiation losses are added from the receiver tube without glass cover(Fig.8).

Solar intensity: The solar intensity is same for both cases whether it is with glass cover or without glass cover .It only depends on weather conditions of a location. HTF outlet temperature: The HTF outlet temperature will be more for with glass cover case as compared to without glass cover because of the convection and radiation losses from the receiver without glass Power consumption of pump: The pump power will be more in case of with glass

cover as compared to without glass cover .This is only due to reason that the mass flow rate will be less to maintain a temperature in case of without glass cover, because less mass flow rate leads to increase in temperature of HTF.

CONCLUSION

Experimental model is developed which is based on thermodynamic analysis of parabolic trough collector. This model is based upon the minimization of radiation losses by the use of triangular cross-section, so that maximum solar radiation can be captured. Also, the use of aluminium metal blocks arrangement in series acted as a long receiver tube under compact glass cover.

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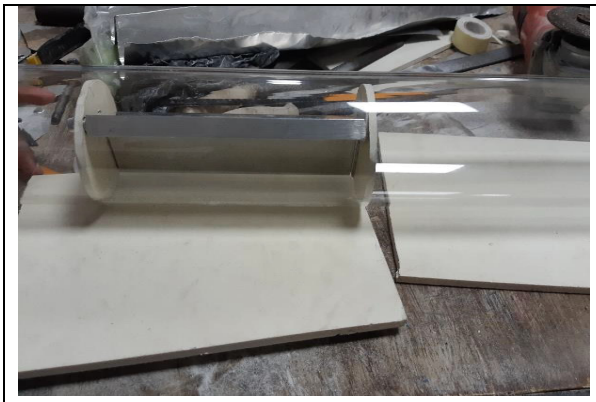

Fig. 1.Glass tube 600 mm length and 90 mm diameter

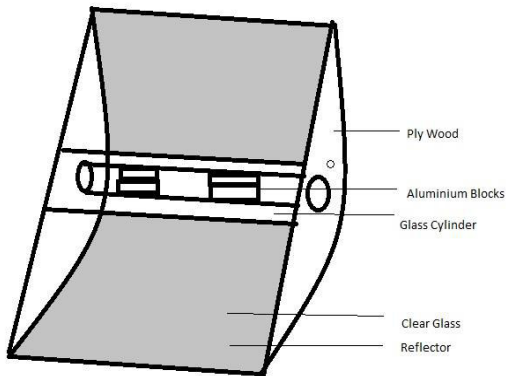

Fig. 2. 2-D view of solar parabolic solar panel

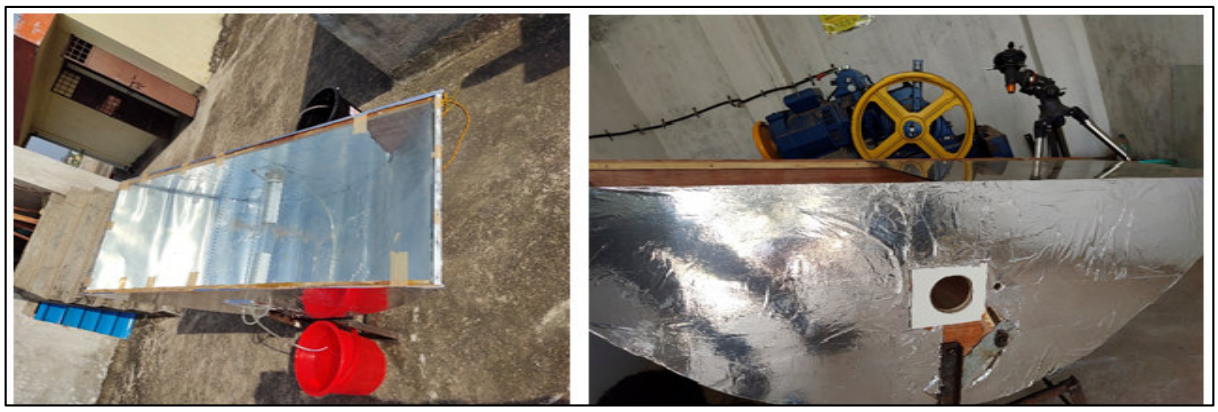

Fig. 3. Experimental setup

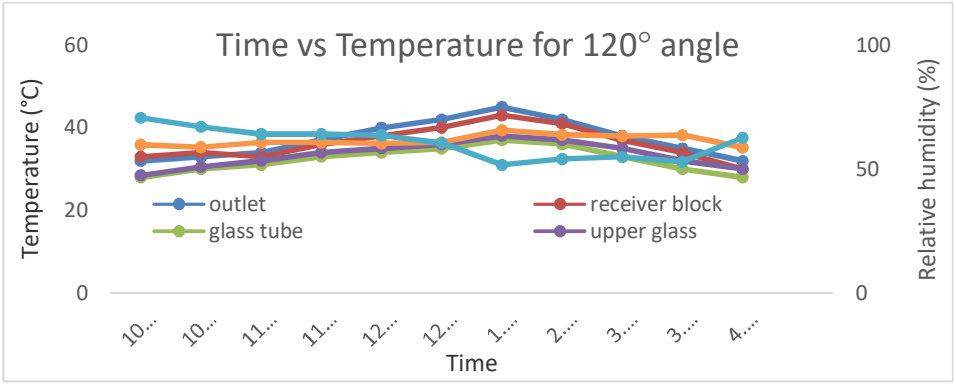

Fig.4.Time vs. Temperature for 120° angle

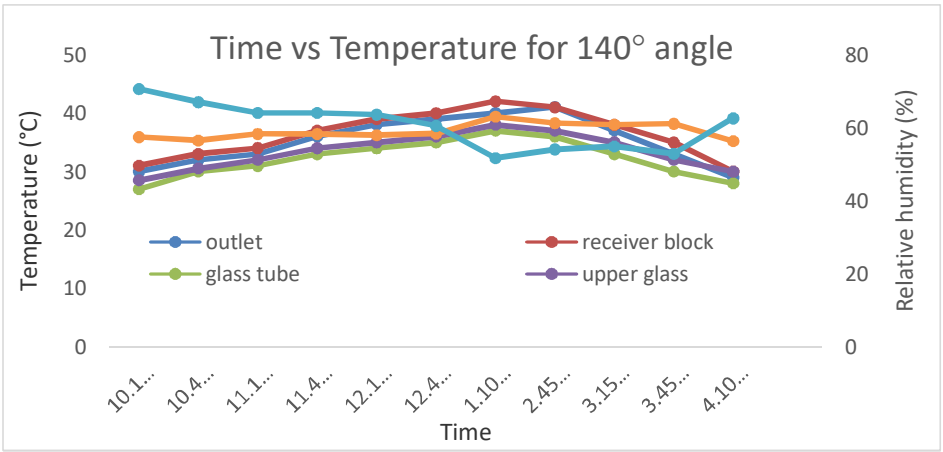

Fig.5. Time vs Temperature for 140° angle

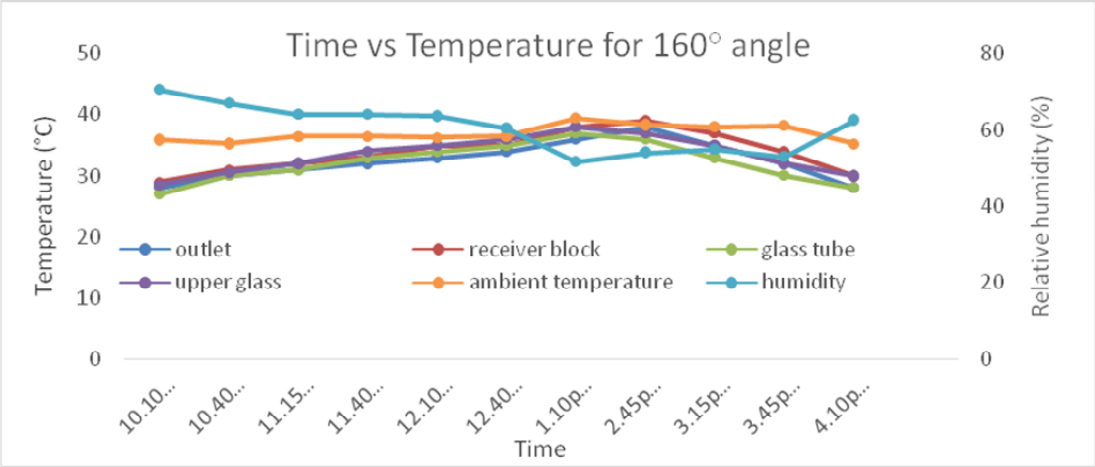

Fig.6.Time vs. Temperature for 160° angle

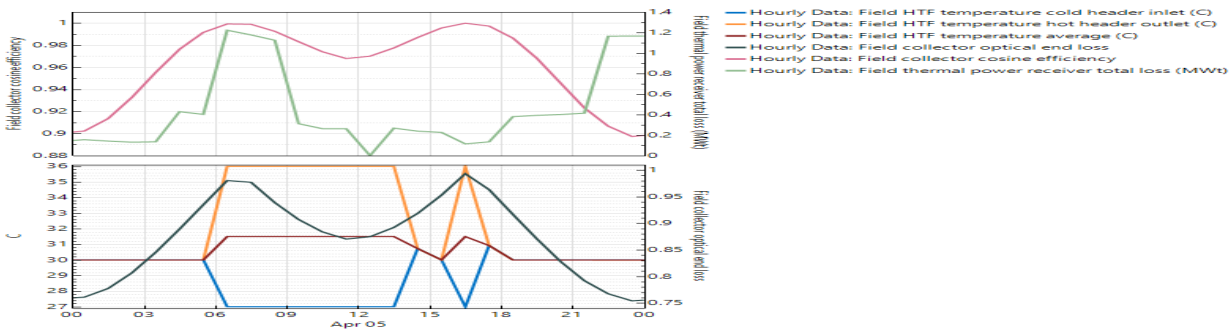

Fig.7. With glass cover

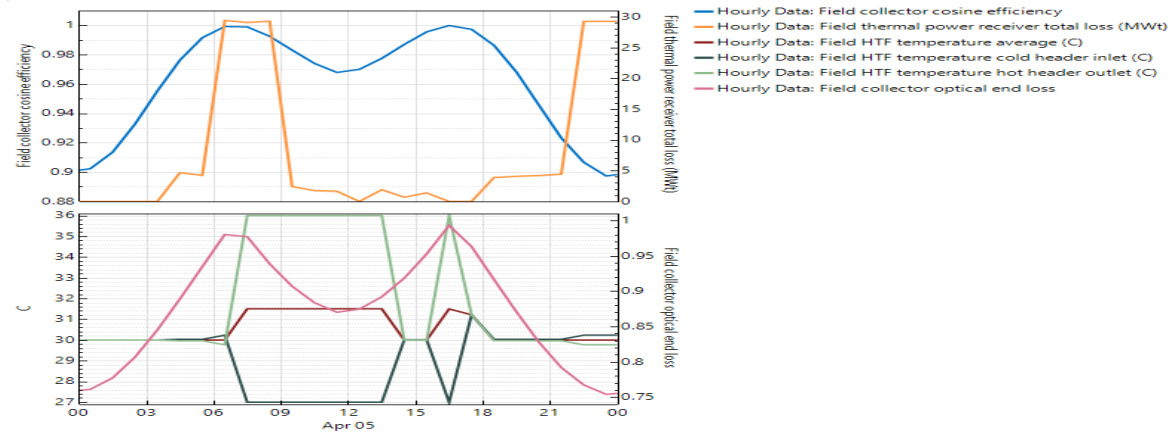

Fig.8.Without glass cover

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RESEARCH ARTICLE

Study of Laminar Flow around the Cylinder

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ABSTRACT

This paper deals with the distribution of velocity, pressure and vortices around the cylinder. It is only a case study of how the flow is distributed around the cylinder. The cylinder is created and then it is exported to the CFD solver; the CFD solver used here uses meshless simulation techniques to solve the problem. The setup and solution of the two-dimensional flow around a cylinder at Reynolds number Red=4000.

Keywords: Flow around the cylinders, laminar flow, simulation of flow, CFD of cylinders,

INTRODUCTION

Create a cylinder Create a cylinder cantered at the origin, in the Z-direction, with radius 0.2 m and height 1.0 m, by means of: Main menu > Geometry > Create object > Create cylinder, or in Toolbar Object Creation. Introduce the geometrical data of the cylinder in the dialogue box (Units in SI):Select the cylinder geometry-object (Shape) either by: selecting the View only in the Toolbar Selection Filter, and clicking either on the cylinder in the Graphic View or on the word Shape in Project Tree > Geometry > Geometries. Once the object is selected, its wireframe is highlighted in blue. selecting the Object filter in the Toolbar Selection Filter, and clicking either on the cylinder in the Graphic View or on the word Shape in Project Tree > Geometry > Geometries. Once the object is filtered, its wireframe is highlighted in blue and the object Gizmos are automatically shown.Rinoshika et al. investigated the flow around the surface mounted short cylinder [1]. Zhang, et al. investigated the effects of the effects of flow around the equispaced four cylinders [2]. Wu et al. investigated the flow around the cylinder under high Reynolds number [3]. Dash et al. investigated the effects of flow around the vertical hollow cylinder [4]. Shi et al. investigated the effects of flow around the D shaped cylinder with an open cavity [5].

Gizmos allow the user to translate, rotate and scale the geometry. To familiarize yourself with gizmos please perform the following actions: click on any of the gizmo axes -the translation dialogue box appears - and enter X = 3 m, Y = 2 m, Z = 1 m. Observe the new position of the cylinder. click on any of the gizmo arch - the rotation dialogue box appears - and enter X = 30 º, Y = 0 º, Z =0 º. Observe the new orientation of the cylinder. click on any the gizmo axes center - the scale dialogue box appears - and enter 2. Observe the new size of the cylinder (twice the original).Make sure that OpenGL mesh deflection = 0.1. If that is not the case, please change the parameter to 0.1, delete the geometry: Select geometry > right mouse button in the Graphic View.Please note: There is no Undo option. Please, save the project frequently.Configure the section Project Tree > Environment > Engine > as follows: (a) Kernel : 2d (b) Flow model: Single phase external (c) Thermal model: Isothermal (d) Turbulence settings: Turbulence model: Automatic Turbulence generation: Off (e) Advanced options: Leave the default setup.

METHODOLOGY

Problem set-up

Environment settings Configure the section Project Tree > Environment > Environment > as follows: (a) Global attributes > Domain type: Virtual wind tunnel
(b) Global attributes > Ext. acceleration laws: leave it to zero
(c) Global attributes > Initial conditions: Wind tunnel default
(d) Global attributes > Reference area: Front
(e) Global attributes > Reference velocity: Automatic
(f) Wind tunnel > Position: move the wind tunnel 2 metres in the +X direction
(g) Wind tunnel > Dimensions: 9 metres length (X), 3 metres height (Y) and 1 metre width (Z)
(h) Wind tunnel > Ground wall: Off
(i) Wind tunnel > Boundary conditions: Velocity
(j) Wind tunnel > Boundary conditions > Velocity law: 10 m s -1 in +X direction.
This boundary condition would be applied on the -X boundary of the wind tunnel (inlet). Materials settings: By default, in single phase external the fluid material is called Gas, which is initialised with the air thermophysical properties. To get a Red=4000, given a fluid velocity of 10 m s -1 and a cylinder diameter of 0.4m, the Gas properties have to be modified as:
(a) Project Tree > Materials > Fluid >Density: 1 kg m -3
(b) Project Tree > Materials > Fluid > Viscosity model: Newtonian.
(c) Project Tree > Materials > Fluid > Viscosity model > Dynamic viscosity: 0.001 Pa s.
Geometry settings: The geometry (cylinder) has been previously created. In the Project Tree, its behaviour and boundary conditions can be defined, as follows:
(a) Project Tree > Geometry > Geometries > Shape: Cylinder > Behaviour: Fixed, leave blank position and orientation.
(b) Project Tree > Geometry > Geometries > Shape: Cylinder > Boundary conditions: Wall, with Automatic wall model and zero roughness.
Simulation settings: Configure the section Project Tree > Simulation > as follows:
(a) Simulation time: 2 seconds.
(b) Time step mode: Fixed automatic (i.e. constant time step).
(c) Time step mode > Courant: 1
(d) Resolution > Resolved scale: 0.04 metres.
(e) Resolution > Refinement algorithm: Disabled (i.e. uniform resolution).
(f) Store data > Folder: Cylinder-test1. This is the name of the folder where the numerical data will be stored.
(g) Store data > Frames frequency: 50 Hz (i.e. frames per second).
(h) Store data > Numerical data frequency: Solver time step, which means any curve plotted in the Function Viewer will be updated at the frequency of the solver steps.

(i) Store data > Save averaged fields: Off
(j) Store data > Save resume file: Off. In case you need to stop and resume your simulation you can switch it to On, however this consumes harder disk space.
(k) Store data > Compute makers: Off. The Graphical User Interface can be closed while the simulation is running. The Process Manager is the minimum interface with your computation. XFlow will reconnect the simulation to the interface by means of the Process Manager when reopening the project. A low stability parameter (< 1) means the stability of the numerical scheme is ensured and the solution should therefore be consistent. If it is very close to 0, you may increase your time step to save computation time. A stability parameter of 1 means the stability of the numerical scheme is not ensured and the simulation may diverge. You must therefore decrease your time step to ensure the convergence. The stability parameter can be monitored in the Function Viewer window. To this end, do right click on the Function Viewer window and select Stability Parameter.

Post processing technique

Create a cutting plane to visualise the velocity field, to do so please go to Project Tree > Postprocessing and do:
(a) Right-click on Cutting planes and select Add cutting plane, or press in the Post Processing Toolbar, or go to Main menu > Post-Processing > Create cutting plane.
(b) Cutting plane > Axis: Select Z (The position of the plane cannot be modified, as it is a 2d simulation)
(c) Cutting plane > Visualisation mode: 3d field.

RESULTS AND DISCUSSION

The velocity distribution around the cylinder can be seen from the Fig.1, it clearly shows that the velocity is maximum at the top and bottom of the cylinder edges. While, the velocity is minimum behind the cylinder.The pressure distribution around the cylinder can be seen from the Fig.2, it clearly shows that the pressure is minimum in the behind of cylinder. Also, fluctuation of high pressures can be seen behind the cylinder back.Fig. 3 shows the vortex distribution around the cylinder, it can be seen that the vortex is maximum at the upper and lower edge of the cylinder.Fig.4 shows the turbulence intensity distribution behind the cylinder, it can be seen that the turbulence intensity is maximum behind the cylinder and at some far distant from it.

CONCLUSION

This can be seen from the above section that the external flow through the cylinder can only be visualized by the CFD. Therefore, it can be applied to different other cylindrical objects under study and this can help to eliminate vortex of bodies in flow. Also, it gives us an idea to remove turbulence in different components under air flowing conditions.

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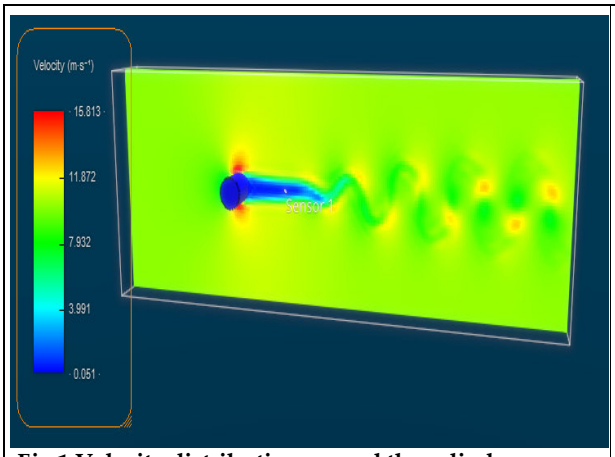

Fig.1 Velocity distribution around the cylinder

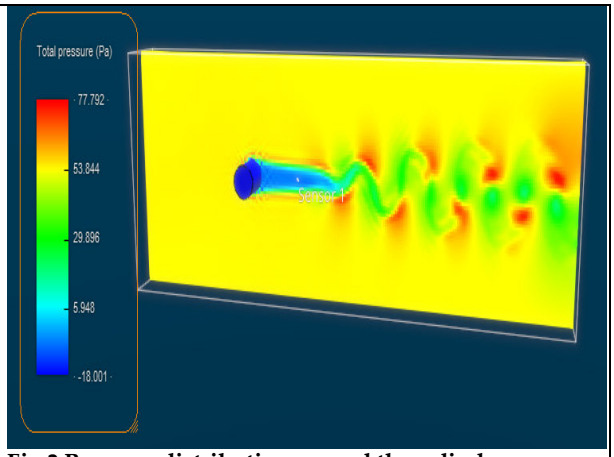

Fig.2 Pressure distribution around the cylinder

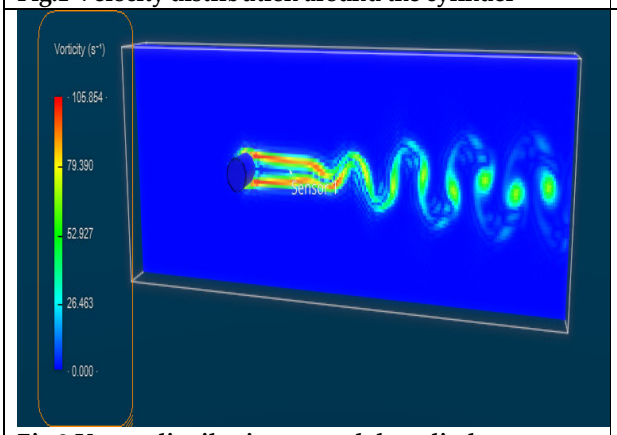

Fig.3 Vortex distribution around the cylinder

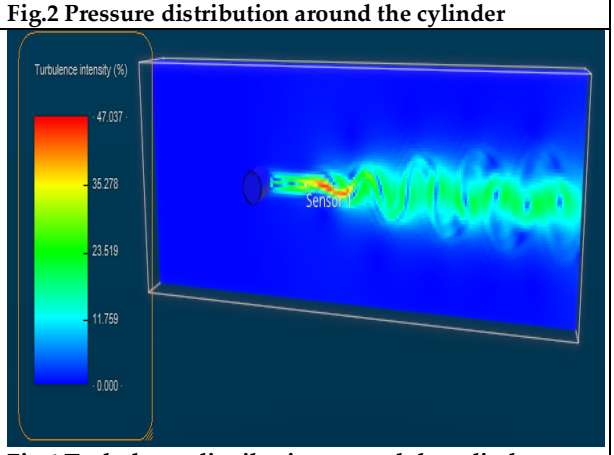

Fig.4 Turbulence distribution around the cylinder

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RESEARCH ARTICLE

Analysis of a Diesel Engine in Dual Fuel Mode with Producer GAS

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ABSTRACT

The energy crisis is a great bottleneck in contribution of energy sources to world economy. Renewable sources are having the ability to offer energy supply for infinite period of time. Electric power generation with bio-mass resources is getting attention all over the world. Diesel and its blend along with producer gas obtained from wood chips in dual fuel mode operation of a diesel-engine may be used as a better option. The present work concentrates on the effect of producer gas flow rates and adding turbocharger on the performance of a twin cylinder dual fuel diesel-engine fuelled with diesel and producer gas. Experiments are done under different loads. Except NO_x and CO_2 emissions, reduction of HC, CO are obtained under turbocharged mode compared to its normal mode at all test conditions.

Keywords: BTE,CO,HC,Turbocharger

INTRODUCTION

Diesel engine offers better fuel to power conversion efficiency in comparison to petrol engines. Growing concern on emission & increase in the cost of petroleum products have put enormous pressure to find alternative sources of fuels as substitute for fossil fuels. So many research works are in progress to develop newer alternative fuels & technology to reduce emission & also help in cleaning up the environment [1, 2].Bedoya et al. have converted the engine to work in dual fuel with a "T" mixture & a mixing length from the intake manifold in first phase and a larger mixing length in second phase. An improved thermal efficiency was found in longer mixing length due to a better mixing of biogas-air, while a reduction in volumetric efficiency was reported due to pressure drop at the inlet manifold[3].Saha et al. performed their experiment on a single cylinder, four-stroke, water cooled diesel engine in dual fuel mode with syngas (mixture of hydrogen and carbon monoxide). A Volumetric efficiency was reduced in dual fuel operation as the inducted gaseous fuel displaces the amount of inducted air into the cylinder [4].

Yoon and Lee observed the performance of the engine with biogas in dual fuel mode. Thermal efficiency of dual fuel combustion for both pilot fuels was lower than normal diesel mode due to incomplete combustion of the gaseous fuel [5].Lakshmanan and Nagarajan changed the engine to work on dual fuel mode with acetylene as gaseous fuel. They found that acetylene injection showed inferior performance than diesel operation at part loads due to formation of lean mixture. But at full load a marginal increase in thermal efficiency was observed because of enhanced suction of gaseous fuel [6].Tippayawong et al. used a 4 stroke single cylinder engine in dual fuel mode where biogas and diesel were taken into consideration. They observed that biogas in dual fuel mode gives a higher power output, brake thermal efficiency as compared to normal diesel operation [7].Banapurmath and Tewari performed the experiment on dual fuel mode with producer gas as inducted fuel and diesel, honge oil, honge oil methyl ester as different pilot fuel. They observed highest thermal efficiency in diesel or producer gas followed by honge methyl ester (HME) or producer gas [8].The effects of gasoline fumigation were found experimentally by Sahin et al. on exhaust emissions and performance of a turbocharged indirect injection diesel engine which results in reduced effective power and increased effective efficiency [9].Gharehghani et al. conducted an experiment to investigate the thermal balance and performance of a turbocharged gas spark ignition engine. Due to increase in engine load and coolant temperature, the % of transferred energy to the exhaust gases was increased and the % of coolant energy decreased [10].

METHODOLOGY

Two different test arrangements for experimental work are conducted in the engine. Test-1 is done by utilising a 4-stroke water cooled twin cylinder diesel engine which is water cooled. The engine is connected with electrical generator and bulb loading devices. A downdraft type biomass gasifier is used for the experiment. Modification of the mentioned engine is made in to turbocharged engine with necessary arrangements. Test-2 is conducted after the necessary changes. A 2500 cc capacity TOYOTA turbocharger with pressure ratio 1.5:1 is used. The turbocharger outlet pressure is more than the engine required pressure after the turbocharger is on. The producer gas induction system experiences back pressure due to high pressure of air. As a result of which, producer gas could not enter into intake manifold. The solution of the problem is to incorporate a flow regulating valve, a y-shaped gas induction system in order to control the air flow. This arrangement gives solution to the gas induction problem as well as a stoichiometric air fuel ratio is maintained. To measure emission parameters, AVL make 5-gas analyzer is used. Under different load conditions varying from 0 to 10 kW, tests are carried out by utilising the Diesel fuel in dual fuel mode. Results are considered by using turbocharger and without using turbocharger.

RESULTS AND DISCUSSION

Brake Thermal Efficiency (BTE)

Fig 1 & 2 reveals the fluctuation of BTE with various loads for diesel in single fuel and dual fuel modes. The result showed that up to 8 kW with increase in load, BTE increases and it decreases for diesel for both modes. Proper combustion happens with rise in load as combustion temperature improves. As a result of this, BTE decreases due to poor combustion at full load condition. In turbocharged mode, BTE for the test fuel is superior than their natural aspirated mode. Due to increase in supply of air by turbocharger, the reaction of air with fuel enhances which results in better Break Thermal Efficiency.

Brake specific energy consumption (BSEC)

With increase in brake power, brake specific energy consumption decreases up to certain value. Slightly increment in brake specific energy consumption compared to turbocharger integration in single fuel mode is shown in the fig 3

and 4.This happens because with increase in brake power, combustion process becomes slow. Combustion process slows down as it gets less time for mixing of fuel-air & higher pressure of inlet air. So it leads to less input energy. As a result of which brake specific energy consumption is reduced.The reason is that turbocharger provides sufficient air for a complete combustion and BSEC decreases.

CO EMISSION

The CO emission fluctuation with loads is indicated in Fig. 5 and 6 respectively for diesel in both test modes. CO emission is reduced in turbo mode of as compared to without turbo mode for diesel in test conditions. Turbocharger gives more oxygen at inlet in full load condition. This results in better combustion indicating lower CO emission. CO emission decreases gradually with increase in brake power and at full load it increases substantially. Due to proper combustion at higher loads the result is obtained. But at full load the fuel richness causes incomplete combustion. Therefore, higher CO emission is observed.

HC EMISSION

Increase in brake power leads to decrease the HC emission to certain value & then increase in both the modes. In single fuel mode HC emission decreases more with using turbocharger, this is because more amount of O_2 is available for complete combustion & increases after that because of slow burning velocity. Hence, due to combustion of incomplete nature; and more load the oxygen percentage in the mixture decreases.In diesel engines, as compared to natural aspirated mode; the turbo operation mode leads to lower emission of HC(fig.7&8). This is only due to efficient and complete combustion of lean mixture which again is due to higher quantity air provided by turbocharger.

CO_2 EMISSION

Fig. 9 & 10 indicates that under different load conditions the emission of CO2 is found to be comparatively more for turbocharger as compared to without turbocharger. This happens because of good oxidation of CO to CO_2. Complete combustion of cylinder charge in turbo mode compared to without turbo mode is responsible for this conversion.CO_2 emission increases due to finer combustion with rise in load.

NO_x EMISSION

The change in NO_x emission at different loads for both test modes is represented in figures. With rise in load, energy input escalates, which out-turns into high combustion temperature. As a result of this, formation of higher NO_x emission is found (Fig. 11 & 12). Turbocharger provides adequate oxygen to the engine.Therefore, higher NO_x compared to natural aspirated mode in both cases of operations are found with turbo charger.

CONCLUSION

The BTE in single & dual fuel mode with turbocharger is 3.73 % & 2.76 % higher than without turbocharger engine with single fuel & dual fuel method respectively. As compared to their natural aspirated mode, the effect of turbocharger indicates a reduction in Brake specific energy consumption, an increase in NO_x emission in dual fuel operation. A decrement of NO_x emission for under test conditions is obtained. The CO_2 emission with turbocharger is higher than without it. With turbo mode, lower emission value of CO, HC are found under all test conditions.

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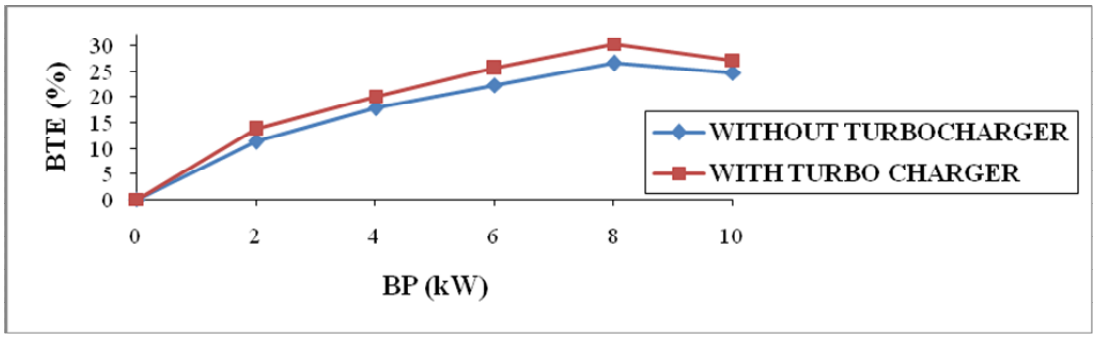

Fig.1.BTE Vs BP with single fuel

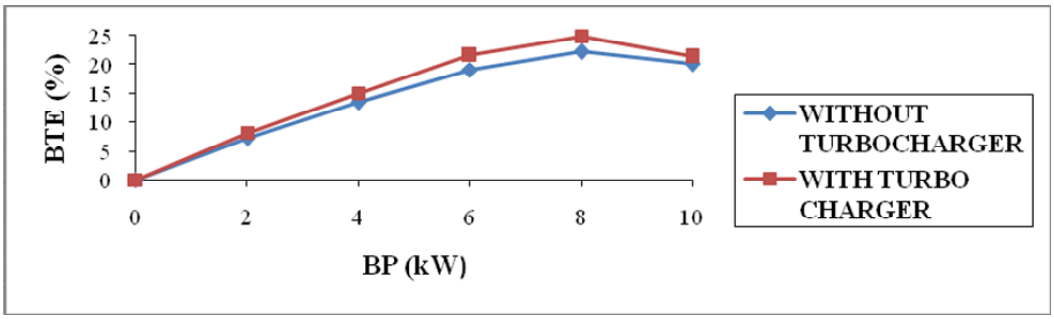

Fig.2 .BTE Vs BP with dual fuel

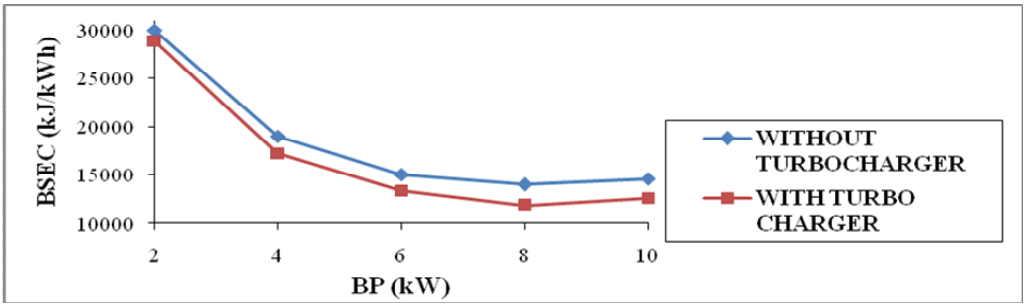

Fig.3. BSEC Vs BP with single fuel

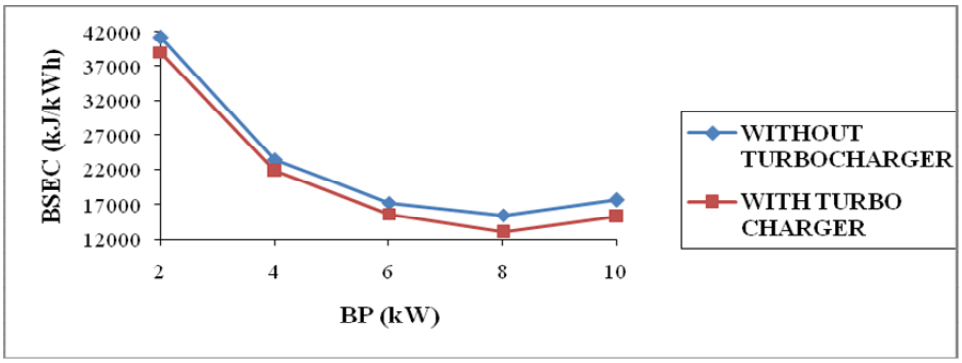

Fig.4.BSEC Vs BP with dual fuel

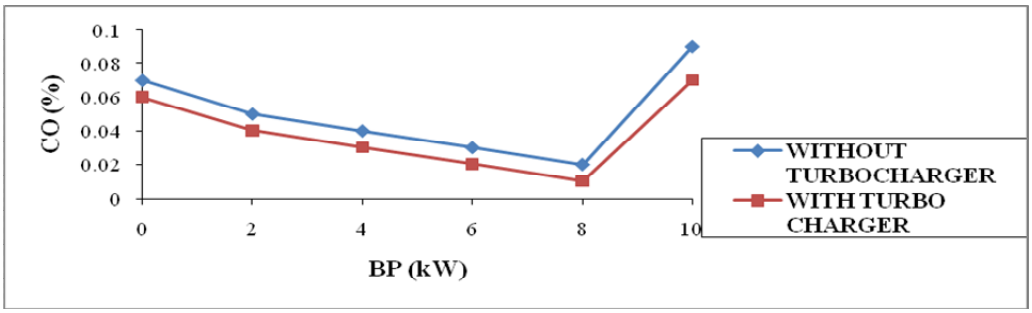

Fig.5. CO Vs BP with single fuel

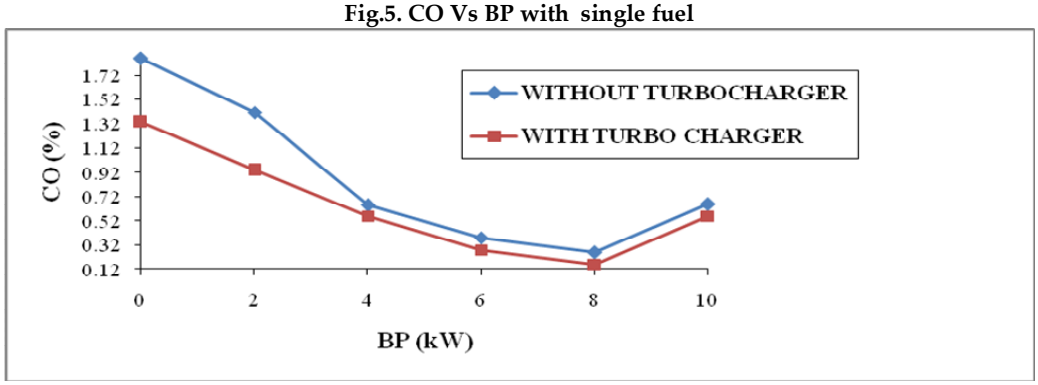

Fig.6.CO Vs BP with dual fuel

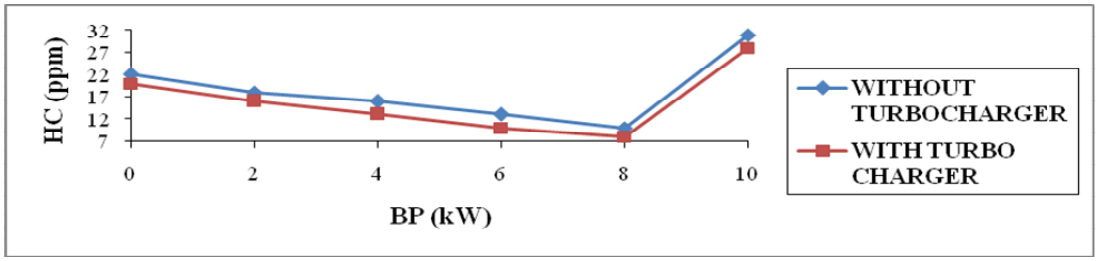

Fig.7. HC Vs BP in single fuel

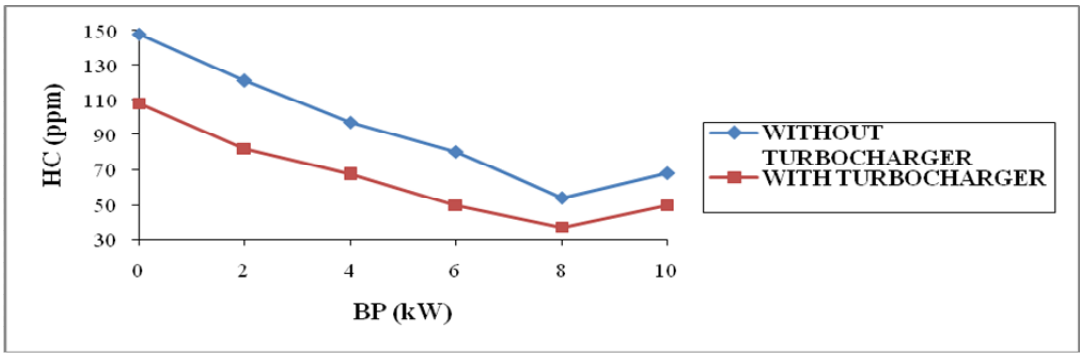

Fig.8.HC Vs BP in dual fuel

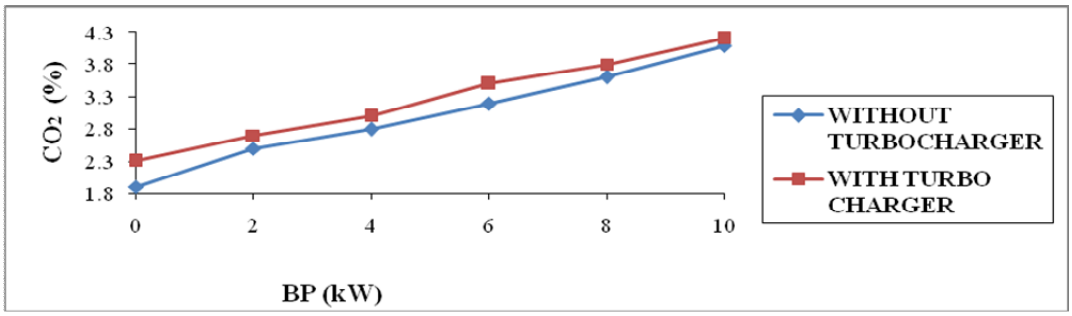

Fig.9. CO2 Vs BP with single fuel

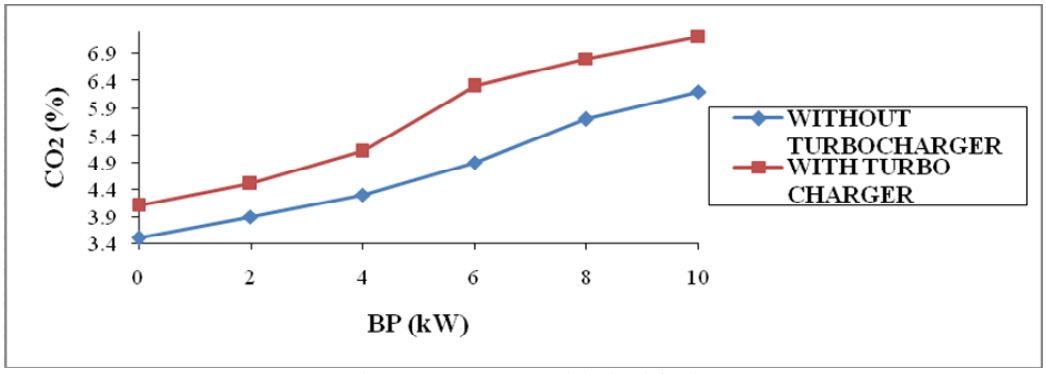

Fig.10. CO2 Vs BP with dual fuel

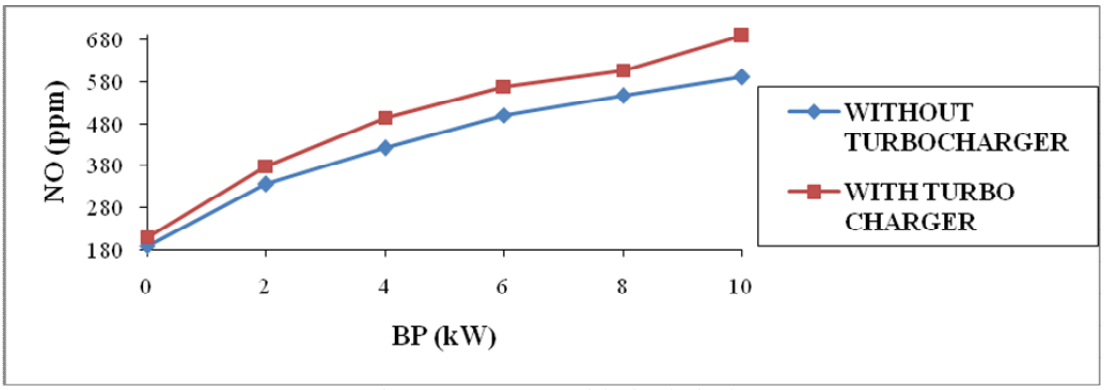

Fig.11.NOx Vs BP with single fuel

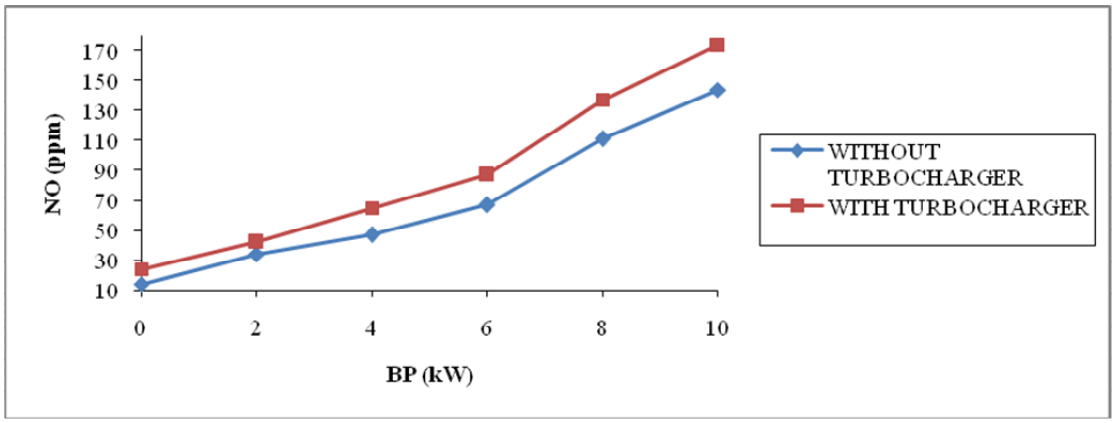

Fig.12. NOx Vs BP with dual fuel

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RESEARCH ARTICLE

Fabrication of Portable Table

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ABSTRACT

In this modern and well equipped world every individual is interested to use articles, tools and equipments which can have numerous functionality and utilization. In this new era people are interested about modern and furnished articles. Earlier due to availability of same and less advancement of engineering world people never focused on multipurpose sources. Due to industrial growth and improvements in engineering field had made it possible to think in new direction. Previously humans are using simple table or rack for their day to activities but now in this new era and development in technologies have given thrust to develop an appliance which can solve the purpose of 3 things at a single time. These considerations motivated us to develop a project which can we used as a ladder, table and shelf. The beauty of this product is, it is space efficient, moveable, easily assembled and dismantled and more over coast efficient. It can be used in offices, Dining room, libraries etc.

Keywords: Multi Purpose Table, Catia, Ansys

INTRODUCTION

In manufacturing Engineering product design has important role in turns of it geometrical parameters like size, shape and its easiness for users. For different purpose people has to buy different product like chair for sitting, dining table for keeping food, drawing table for drawing sheets, etc. But our project is design to use a single universal table for fulfilling multiple purposes in a single product. This table would help the individual in many different way like first of all the main thing money, it is of low cost as compare to the cost of the entire thing which it will provide. So indeed it is a money saver. Other thing it is durable hence no requirement of replacement of the whole table[1,2,3].A study was conducted to realise the lifestyle, need and comfort in the Indian homes as well as different activities associated with specific interiors. Drawings were developed for final concept, and designed using Catia and analyzed using ANSYS software [4].

In India majority of Indian middle class populations are living in small flats because of their economy scale as well as the lack of space availability for living. To overcome this problem the various arrangements of the furniture should be multipurpose, space saving than their primary functions[5].Space saving furniture is one of the options to solve these problems.Introducing the innovative designs, the hard wares, the application and future development, cost & price and the important market of transformable space saving furniture[6].

In the field of manufacturing engineering product design plays a key role in turns of it geometrical like size, shape and its easiness for users. But in this paper we have to design a single universal table for fulfilling multiple purposes in a single product. Multipurpose wooden table is a table which can transform into tool, chair, comfort chair, tea table, centre table, Tea table, drawing table and dining table and this is achieve with the help of different mechanical linkages such as spring return, sliding joints ,hinges, etc. To prepare our product the type of material should be properly selected considering design, safety and strength.

1. Wood: wood is readily available in market. It is economical. It is light in weight and easily machined. Hence it is good for portability.
2. Brass: Has good mechanical properties. It is corrosion resistance.
3. Mild steel: It has high tensile strength. It is economical and available in standard sizes.

Multi-Purpose table for furnishing

A multi-purpose table for furnishing is anticipated, comprising: a top with a thickness and perimeter edges delimiting a Support Surface of the top' Supports on the underside of the top, a clearance aperture passing through the top and developing in such a way as to interrupt both the support surface and perimeter edges, a mobile element counter-profiled to the clearance aperture and aimed at re-forming the support surface and perimeter edges, and fixing means between the top and mobile element to constrain the mobile element in a removable Way in the clearance aperture.

OBJECTIVES

General objectives

1. To study the existing design of Table considering ergonomics concept: while surveying the market, we have designed a table that will consume less efforts of the human and will yield with the multiple functions in a single table. Aesthetically this project is designed, so that the individual using it will feel comfortable.
2. To study the enhancements in design and modifications in existing design: after the market survey we have accomplished a design of a table that can withstand with varieties in a single table.
3. Modelling and simulation of table design for stress Analysis: for the purpose of modelling we have used Catia software and for stress analysis we have used ANSYS-19.2.
4. Fabrication of Table : with the help of above described surveying points ,we concluded to design a table that will work with multi functionality i.e. chair, ironing table, tea table, easy chair, centre table, drawing table and dining table, it took lot of efforts to tackle the obstruction while designing this particular table.

Specific objectives

1. To plan the table structure.
2. To design different parameters related with the mechanical linkages and structure.
3. To make it available at lower cost.
4. To implement the manufacturing processes for creation of the sub-components.

5. To assemble the subcomponent and check the reliability of the creation.
6. To test the product whether it is performing the intended task.

MATERIALS AND METHODS

Project Flow

This section will explain about the flow or step involved in designing the concept. Basically, the project flow (fig.1) is as below:

I. Identify the problem statement and find the solution
II. Concept design and evaluation
III. Finalize concept
IV. Material selection
V. Fabrication process and finishing

From the flow chart below, this project starts off with literature review about the project title. After finishing the literature review, it is moved to process of identifying the problem that is being faced by the customers. Market surveys about the existing product were completed. Before coming out with concepts, objective and scope of the project was determined so that the process of concepts generation will be easier and more effective. After that, five concept designs (fig.2)were made and then the analysis was done with these concept designs. Method of concept screening is using to finalize concept. After final concept was chosen, it will be draw by using Catia software and dimension was given. After the final concept and material selection has been identified, Ansys (19.2) software is using to do analyze structure on final concept. After analyzing structure, the fabrication is proceeded to fabricate the final concept. Cutting, welding, drilling, filling and finishing process was conducted in fabrication process. After fabrication the final concept, testing process on the product was done (fig.3).

In project work we fabricated our product by the help of drilling, boring, reaming, welding, cutting the material as per required dimension and also color our product. The main raw material we used is mild steel. The other materials screw, wheel for easy transfer from one place to another, ply wood, clamp, drilling machine, welding is done by arc welding process.

Material

When we planned to make portable table cum shelf the main thing that it was analyzed which material is convenient for this product. That material should light in weight, cheaper in price; easily transfer for one place to another. For analysis all the information we are planed that mild steel is suitable for this.

Cutting of Material

When we are manufacturing our product it is bound that we have to cut the material as per our requirement. We cut mild steel for the base as it gives strength to the structure. We cut 2 piece of same size for side support and a long horizontal .Then we made 5 set of self where we have to cut 2 piece of height and2 piece of breadth of each. Then for support two side 4 supporting bar is required.

Grinding

After cutting the material with required dimension we notice that some junks are attached with our material. For removing this product some operation is required i.e.grinding.In grinding operation the rust got removed. The

grinding is done by drilling machine. Grinding tool is fitted in drilling machine. Now the material is ready for fabricated.

Boring

When the material is grinded then we finished the boring and drilling operation. We made hole in lower part for the fixing of base and wheel. Then we dilled in side supporting bar for the fixing of plate and make the product strong. Drilling is done by sane position and same distance. After drilling done we finished the drill hole by the help of boring reaming.

Welding

All the boring and grinding operation is done then we go for welding. Then we welded part of the lower part that is called base. When base is completed then we fixed the one part of each side .Then we weld the other part of side base and it is fixed with other side base. We welded the clamping .Now welded the 5 set of rack with same size with length.

Assembly

After completion, we made assembly of all the part in our lab. First we assembled the base part with the help of welding. Then we fixed the side part and place the rack size in product. After all the assembly the final product is ready.Now the product is ready after completion of all these process. Now we are going for load test. When all this completed, the final product (fig.4)is ready to go for market for selling.

CONCLUSION

Transformable space saving furniture is an innovative product. It got opportunity for future development and a huge market. Transformable space saving furniture provides small properties with greater space and multiple functions. Its designs could be combined with the structures and layouts of buildings, so that the functions of both the furniture and buildings could be maximized. In order to improve the future of transformable space furniture, its designers need to create more innovative ideas, and cooperating with architects and engineers is another way they might achieve success. Lowering overhead costs and furniture prices is another element for serious consideration.

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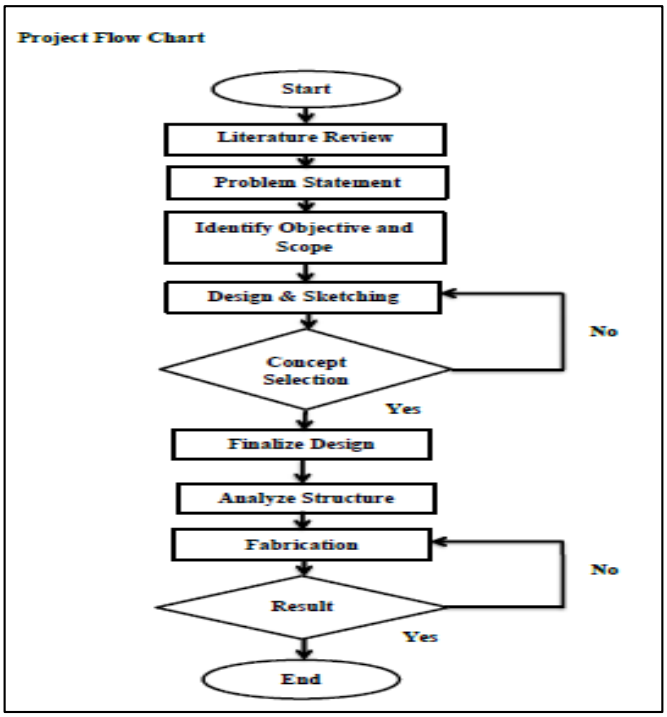


Figure 1. Project Flow Chart

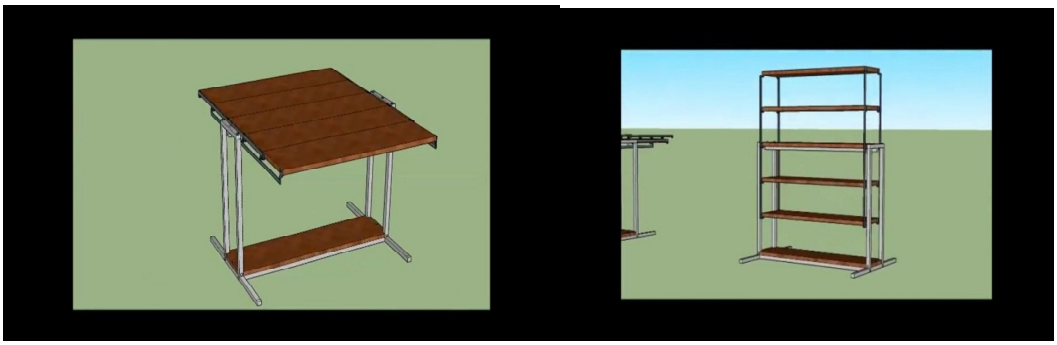
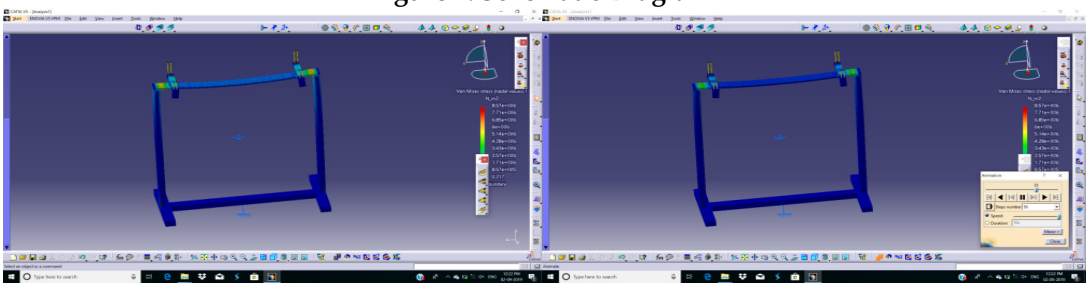


Figure 2. Schematic Diagram



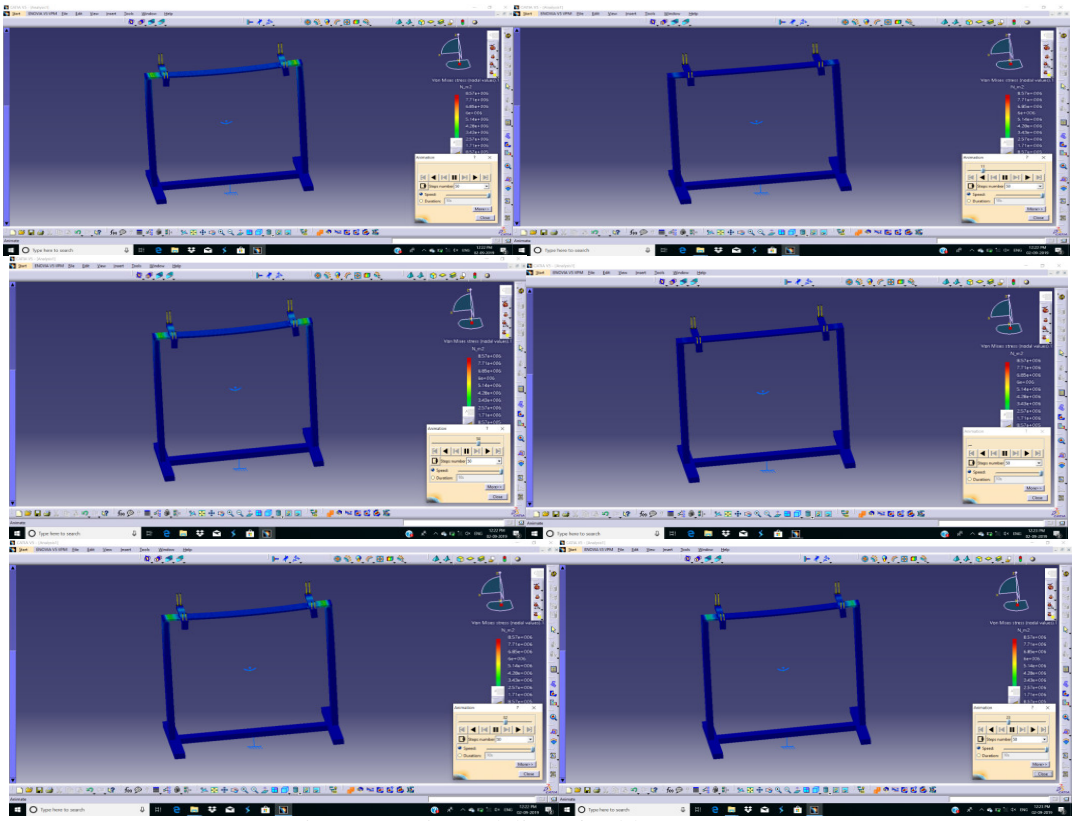


Figure 3. Catia Modeling of Table structure

Figure 4. Final Product

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RESEARCH ARTICLE

Experimental Analysis of Cabinet Type Solar Dryer using Evacuated Tube and Thermal Energy Storage Device

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ABSTRACT

The performance of the dryer was enhanced by the use of evacuated tubes incorporated with PCM and later on its performance was increased by transformer oil filling in the annular space between the glass and the copper tube. The performance of the dryer was seen to be in the order of Black Plate Collector Free mode, black plate collector forced mode, evacuated tube + PCM free mode, evacuated tube + PCM forced mode, oil + PCM free mode, and oil + PCM forced mode. The drying efficiency was seen to be increasing for chilli and ginger respectively. The mean peak collector efficiency for black plate, evacuated tube + PCM mode and oil + PCM mode were seen to be increasing in free convection mode and forced convection mode. Also, the temperature at desired points was seen to increase in the order of increased performance. As the dryer chamber temperature were seen to be in the increasing order of 57, 58, 62, 63, 68 and 71 for Black Plate Collector Free mode, black plate collector forced mode, evacuated tube + PCM free mode, evacuated tube + PCM forced mode, oil + PCM free mode, and oil + PCM forced mode respectively. The numbers of days are reduced from 5days to 1 and half day, where 5 days are required for black plate free mode whereas 1 and half day is required for oil +PCM forced mode. The temperature from 5pm to 6pm are seen to remain constant, this was only due to use of PCM (paraffin wax). So, on the whole the solar cabinet dryer performance was increased.

Keywords: Evacuated Tube, PCM, TES

INTRODUCTION

Solar Energy will be going to be 5th generation main energy sources with its easy availability and scarcity of non-renewable energy sources. With increasing demand of energy sources to harness our daily needs and scarcity of coal

and petroleum products it will be a better option to depend upon more reliable renewable energy sources. Various research works are going on solar energy but it still many more to be done to fully depend upon its utilization.Drying is defined as a process of moisture removal due to simultaneous heat and mass transfer. It is a classical method of food preservation, which provides longer shelf-lighter weight for transportation and small space for storage.Hossain and Bala used a mixed mode type forced convection solar tunnel drier to dry hot red and green chillies under the tropical weather conditions of Bangladesh. Moisture content of red chilli was reduced from 2.85 to 0.05 kg kg^{-1}(db.) in 20 h in solar tunnel drier and it took 32 h to reduce the moisture content to 0.09 and 0.40kg kg^{-1}(db.) in improved and conventional sun drying methods respectively. In case of green chilli, about 0.06 kg kg^{-1}(db.) moisture content was obtained from an initial moisture content of 7.6 kg kg^{-1}(db.) in 22 h in solar tunnel drier and 35 h to reach the moisture content to 0.10 and 0.70kg kg^{-1}(db.) in improved and conventional sun drying methods respectively[1].Chowdhury et al. presented an energy and exergy analysis of solar drying of jackfruit leather in solar drying of jackfruit leather in a solar tunnel dryer. Jackfruit leather was dried from an initial moisture content of about 76% (w.b.) to 11.88% moisture content (w.b.) in the solar tunnel dryer within 2 days of drying while at the same drying time the moisture content of similar sample reached 13.8% (w.b.) in the open sun drying method[2].Kaewkiew et al. investigated the performance of a large-scale greenhouse type solar dryer for drying chili. It was found that five hundred kilograms of chili with the initial moisture content of 74% (wb) were dried within 3 days while the natural sun dried needed 5 days [3].Ceylan and Ergun found out the relation between the psychometric working upon the thermo- dynamic analysis of humid air and drying at a timber dryer was investigated [4].Singh conducted an experiment on the thin layer silk cocoon drying in a forced convection type solar dyer. The cocoon was dried from the initial moisture content of about 60–12% (wb) [5].Hii et al. investigated the kinetics of heat pump drying of cocoa beans under stepwise drying conditions and the heat and mass transfer analysis was carried out using 3-D computer simulation [6].Sallam et al. used two identical prototype solar dryers (direct and indirect) having the same dimensions to dry whole mint.The values of the effective diffusivity coefficient for the mint drying ranged between $1.2\times 10^{-11}$and 1.33×10^{-11} m^2s^{-1} [7].Mette et al.performed their research in the field of long-term thermo chemical energy storage for low temperature application (e.g. solar thermal systems).). In this paper, an overview of research activities carried out at different national and international institutions related to long-term thermo chemical energy storage for solar thermal applications was studied [8].Yang et al.designeda solar air heater with offset strip fins which was optimized by numerical modelling. Results indicated that the instantaneous thermal efficiency exceeded 0.40 when the heater was running at low airflow rate(100 m3 h^{-1}) ,solar irradiance on the collecting area was 600Wm^{-2}, indoor air temperature 14°C, outdoor air temperature -5°C, and solar incidence angle20° [9].Cuypersa et al. developed a seasonal thermo chemical storage system for dwellings and offices[10].

Kumar et al. presented the results of an experimental investigation of heat transfer and friction in the flow of air in rectangular ducts having multi v-shaped rib with gap roughness on one broad wall [11].Chabane et al. investigated experimentally the thermal performance of a single pass solar air heater with five fins attached. A comparison of the results of the mass flow rates by solar collector with and without fins showed a substantial enhancement in the thermal efficiency [12].Kasperski and Nem performed the experiment on a thermo-hydraulic analysis of a solar air heater with an internal multiple-fin array. Proposed multiple fin-array technology enables to decrease the demanded air flux of 7 to10 time incomparison to the smooth pipe arrangement of the absorber. Even with the flux decreased, the efficiencyof internal multiple-fin array arrangement was higher than the one available for smooth pipe arrangement [13].Sole et al. highlighted the parameters to take into account previous to the design of thermal energy storage [14]. Neises et al. performed the experiment on thermal energy storage (TES) which will improve the efficiency and output of solar power plants [15].Block et al. presented an experimental study on the cobalt-oxide/iron-oxide binary system. Compositions of around 10% iron-oxide were identified having appropriate enthalpies and being beneficial in terms of micro structural stability [16].

Several methods have been used to improve the performance of different types of dryer with the help of investigation on various performance parameters like moisture content, drying rate, drying efficiency, collector efficiency and temperature increment at desired points. Also, different crops have been dried to see what will be the effect of drying parameters for different types of dryer used for drying purposes.

OBJECTIVES

- To analyse the performance of the solar cabinet dryerfor chilli in both free and forced mode.
- To modify, design, manufacture and analyse the performance o fsolar cabinet dryer using evacuated tubes by considering the same collector area for chilli
- To modify and analyse the performance of solar cabinet dryer with evacuated tubes for nocturnal use by using the heat storage medium.
- To analyse the performance of evacuated tubes in the solar cabinet dryer by filling the transformer oil in the annular space between the glass and copper tube.

METHODOLOGY

Experimental Setup before Modification

The schematic diagram of the experimental setup is shown in Figure 1.The solar dryer we had used in our experiment is of cabinet type solar dryer. The design of the solar dryer is based on the climatic conditions of the place, nature of the product and the quantity of the product to be dried. The indirect type of the solar dryer was designed and constructed and then it was coupled with already available solar collector. The dimension of the solar collector is 1.55 by 1.09 m. The dryer is of 0.6m height from the ground, the inlet ambient air enters through the inlet of the collector of square cross-section having dimension of 12cm by 12cm. After that the inlet air is heated up with the help of solar air collector and the outlet is connected to the solar dryer inlet, where the hot heated-up air carries out the moisture content of the product to be dried and the extra moisture carried by the air is then thrown by the outlet of the drier. The electric blower used here have a capacity of 379W, as already mentioned the capacity of the drier is of 2kg of raw product. Matt black paint is used on the absorber plate to increase the absorptivity to solar radiation. The collectors were oriented due south at an angle of 45°. A 1000W auxiliary heater was constructed from a galvanized steel sheet with a square cross section area that had a slide length of 0.27m; heating filament was wrapped on ceramic isolators. A constant variable resistance is provided to control the output power required to provide the selected air inlet temperature to the drying chamber. The power is calculated from the reading of the voltage provided by the variac and the amperage read by a digital multimeter (type ID-1000, range: 0-30 A and accuracy 0.75). An aluminum drying chamber, which had the dimension of 1.05 ×0.5 ×0.9m (length × width × height) was insulated from the outside by a 30-mm aluminum coated rock wool sheet. 8 numbers of trays are inserted in the dryer. The drying of the materials involve the migration of water from the inner of the material to its surface, and then removal of the water from the surface; which in turns requires an equivalent of latent heat of evaporation of water.

Dryer Modification

The dryer was modified by implanting evacuated tube above the black plate collector (fig.2) incorporating with PCM (Paraffin Wax) as the heat storage medium behind the black plate. This in turn has increased the performance of the dryer. After that, oil was filled in the annular space between the copper and the glass tube by mixing it with carbon graduals. The mixture was a semi solid type of slug which acts as a conducting medium between glass and copper tube. The performance of the dryer was seen to be increased surprisingly.

Solar Cabinet Dryer Observation Procedure

Step- 1: About 2 Kg of sample weight of chilli or ginger was taken from the local market of Bhubaneswar having the initial moisture content of 88.5-90%.
Step- 2: The sample was placed in the trays of the dryer and its door was closed properly.
Step- 3: The thermocouples was attached at all the desired points where the temperature was required to be measured; such as inlet to the collector, outlet of the collector, inlet to the dryer, dryer inlet temperatures (lower shelf temperature, upper shelf temperature and mean temperature of the dryer), collector plate temperature and the ambient temperature. The temperature was measured from 8 in the morning to 6 in the evening for an interval of an hour.
Step-4: The anemometer was used to measure the velocity of wind at the inlet for both in case of free and forced modes. Also solar power meter was used to measure solar intensity simultaneously for each and every reading that was taken for the measurement of temperature and wind speeds. Also, hygrometer was used for the measurement of humidity both at the inlet of the dryer and to its outlet.
Step-5: After each interval of an hour weight of the sample was measured and from back calculation moisture contained during each interval of an hour was calculated.
Step-6: The readings were taken for both natural and forced mode.

RESULTS AND DISCUSSION

Variation of Moisture Content with time

The graph of Fig.5.2 & Fig.5.3 shows the rate of decrease of moisture content for different modified and unmodified modes of the dryer. As the graph is seen steeper from black plate free, black plate forced, evacuated tube with PCM free, evacuated tube with PCM forced to oil with PCM free and oil with PCM forced respectively, it is cleared that the rate of decrease of moisture content of the sample is higher for oil with PCM forced and is lowest for the black plate free mode,the moisture content was reduced from about 88.5 to 7 %. This is only due to reason of high heat addition which in turn increases the drying chamber temperature, which leads to increase in moisture removal rate respective consequent cases.

Variation of Drying Rate with time

In this graph of Fig.5.4& Fig.5.5the drying rate was seen to be higher for oil with PCM forced and will be seen to be decreased to black plate free mode. The drying rates for the case of chilli for different cases were seen to be in the range of 12.4 kg/ hr, 13.55 kg/ hr, 15.45 kg/ hr, 17.9 kg/hr, 24.35 kg/ hr, and 35.4 kg/hr respectively; whereas for the case of ginger it was seen to be in the order of 14.05 kg/ hr, 14.6 kg/ hr, 15.3 kg/ hr, 18.05 kg/ hr, 28.5 kg/ hr and 40.15 kg/ hr for consequent cases. This was only due to reason of high heat addition to the drying chamber, which in turn had increased its temperature and hence the efficiency. Latter on the bars were seen to be staggered and modulated upon one another, this is due to the fact that at the latter stage of drying there will be very less moisture content in the drying sample and for that there will be almost no or very little differences in the drying efficiency of the dryer for different modes. This is because, for very less moisture content within the sample all the modified and unmodified versions have almost no effect on the drying rate.

Variation of Drying Efficiency with time

The graph of Fig.5.6 & Fig.5.7below shows that the efficiency of the oil with PCM forced mode version of the dryer is the highest and it goes decreased to black plate free version.The performance of the dryer was seen to be in the order of Black Plate Collector Free mode, black plate collector forced mode, evacuated tube with PCM free mode, evacuated tube with PCM forced mode, oil with PCM free mode, and oil with PCM forced mode. The drying efficiency was seen to be in the order of 25.52%, 27.88%, 31.78%, 36.83%, 50.102% and 72.838%respectively for

chilli; where as in case of ginger it was observed in the order of 28.90%, 27.05%, 31.48%, 37.139%, 58.64% and 82.611% respectively.This was only due to reason of the fact that the conversion of energy from solar intensity to heat had been improved in the consequent cases. At the latter stage the curves are seen to be staggered and cover one upon the other, this happens due to the fact that at that stage the moisture content of the sample was so low that it doesn't matters over an interval of an hour for the increased in efficiency. This is because at the latter stage almost maximum % of the moisture has been evaporated.

Variation of Collector Efficiency with solar shine hours

The collector efficiency of the dryer was seen from the graph Fig.5.8 to be higher for in case of oil with PCM forced mode and it goes on decreased for black plate free mode. The mean peak collector efficiency for black plate, evacuated tube with PCM mode and oil with PCM mode were seen to be in the increasing order of 8%, 9.15% and 10.467% respectively in free convection mode; where as it was seen to be in the order of 22.47%, 25.34% and 29.451% respectively in forced convection mode. The graph is seen to be monotonically increased up to 1 pm in noon and goes to monotonically decreased up to 6 pm in the evening, this happens only due to reason that solar intensity of the radiation goes on increasing from 8 am in the morning to the noon and is highest at 1 pm in the noon and again then goes decreased to 6 pm in the evening.

Temperature Variation at Desired Points

The given figures of temperature variation show the various temperatures at the desired points in the dryer. Ambient temperature is the lowest and the collector plate temperature is the highest. The temperature at desired points was seen to increase in the order of increased performances. As the dryer chamber temperature were seen to be in the increasing order of 57℃, 58℃, 62℃, 63℃, 68℃ and 71℃ for black plate collector free mode, black plate collector forced mode, evacuated tube with PCM free mode, evacuated tube with PCM forced mode, oil with PCM free mode, and oil with PCM forced mode respectively. In the six above temperature graphs we can see that the temperature at the desired points will going to be increased for its each modified version, that means the temperature curves are seen to be increased from black plate free to forced then to evacuated tube free and then to forced and subsequently to oil free to its forced version.The only reason to above statement is due to increase in drying efficiency, the conversion of radiant energy to heat energy had been increased which is a clear sign of increase in temperature at desired points for the consequent cases. From Fig.5.10 to Fig.5.14 we can see that the temperature at the desired points are remained to be almost constant from 5 pm to 6 pm and this was due to PCM used that tried to maintain constant temperature after the sunset.

Variation ofHumidity at Desired Points

The Fig.5.15 shows that relative humidity at outlet is greater than relative humidity at inlet; this is due to the fact that moisture addition to the inlet humidity occurs inside the drying chamber. Also, the humidity at outlet for different consequent cases such as black plate free mode, black plate forced mode, evacuated tube with PCM free mode, evacuated tube with PCM forced mode, oil with PCM free mode and oil with PCM forced mode were seen to be increased at each instant of time, as 65.9%, 75.4%, 77%, 81%, 84%, 86% and 88% at 10 am respectively. This was only due to high moisture removal rate for consequent modified cases, as there had been an increase in the moisture content of air inside the drying chamber due to higher efficiency of the dryer.

CONCLUSIONS

The dryer was modified by keeping the collector area constant andthen implanting evacuated tube above the black plate collector incorporating with PCM(Paraffin Wax) as the heat storage medium behind the black plate. This in turn has increased the performance of the dryer. After that, oil was filled in the annular space between the copper

and the glass tube by mixing it with carbon graduals. The mixture was a semi solid type of slug which acts as a conducting medium between glass and copper tube. The performance of the dryer was seen to be increased surprisingly.

- The performance of the dryer was enhanced by the use of evacuated tubes incorporated with PCM and latter on its performance was increased by transformer oil filling in the annular space between the glass and the copper tube.
- The drying rate was seen to be higher for oil with PCM forced and will be seen to be decreased to black plate free mode. The drying rates for the case of chilli for different cases were seen to be in the range of 12.4 kg/ hr, 13.55 kg/ hr, 15.45 kg/ hr, 17.9 kg/hr, 24.35 kg/ hr, and 35.4 kg/hr respectively.
- The performance of the dryer was seen to be in the order of Black Plate Collector Free mode, black plate collector forced mode, evacuated tube with PCM free mode, evacuated tube with PCM forced mode, oil with PCM free mode, and oil withPCM forced mode.The drying efficiency was seen to be in the order of 25.52%, 27.88%, 31.78%, 36.83%, 50.102% and 72.838 respectively for chilli; where as in case of ginger it was observed in the order of 28.90, 27.05, 31.48, 37.139, 58.64 and 82.611 respectively.
- The mean peak collector efficiency for black plate, evacuated tube with PCM mode and oil with PCM mode were seen to be in the increasing order of 8%, 9.15% and 10.467% respectively in free convection mode; where as it was seen to be in the order of 22.47%, 25.34% and 29.451% respectively in forced convection mode.
- Also, the temperature at desired points was seen to increase in the order of increased performance.As the dryer chamber temperature were seen to be in the increasing order of 57, 58, 62, 63, 68 and 71 for Black Plate Collector Free mode, black plate collector forced mode, evacuated tube with PCM free mode, evacuated tube with PCM forced mode, oil with PCM free mode, and oil with PCM forced mode respectively.
- The humidity at outlet for different consequent cases such as black plate free mode, black plate forced mode, evacuated tube with PCM free mode, evacuated tube with PCM forced mode, oil with PCM free mode and oil with PCM forced mode were seen to be increased at each instant of time, as 65.9%, 75.4%, 77%, 81%, 84%, 86% and 88% at 10 am respectively.
- The numbers of days are reduced from 5days to 1 and half day, where 5 days are required for black plate free mode where as 1 and half day is required for oil with PCM forced mode.
- The temperature from 5pm to 6pm are seen to remain constant, this was only due to use of PCM (paraffin wax).

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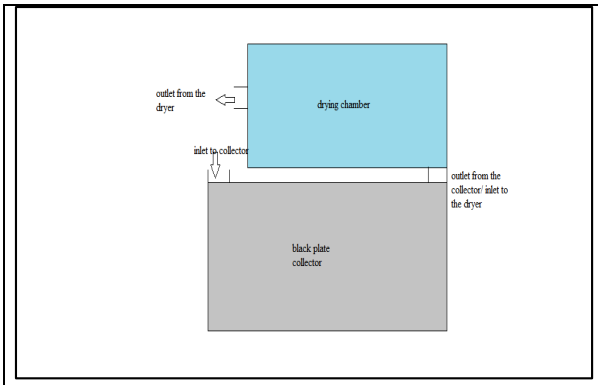

Fig.1.Schematic diagram of the setup before modification

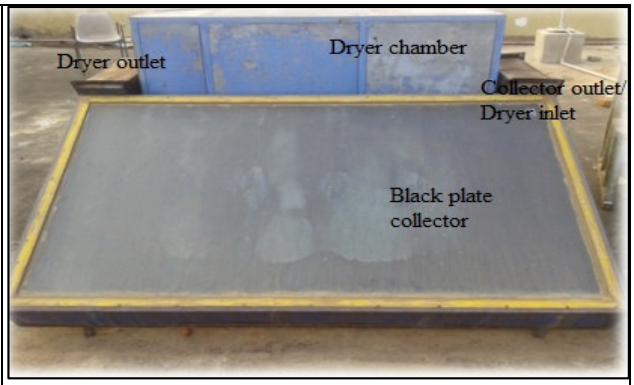

Fig.2.Solar cabinet dryer with black plate collector

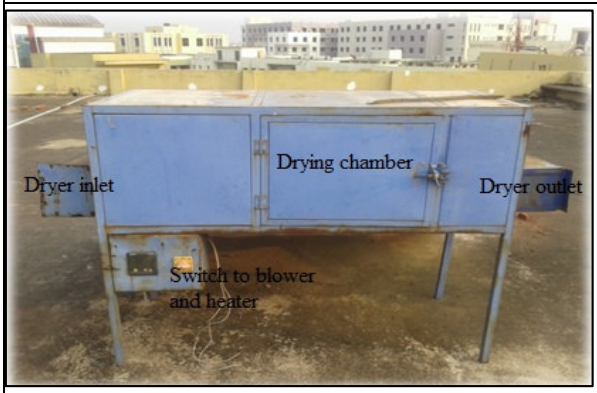

Fig.3.Solar cabinet dryer

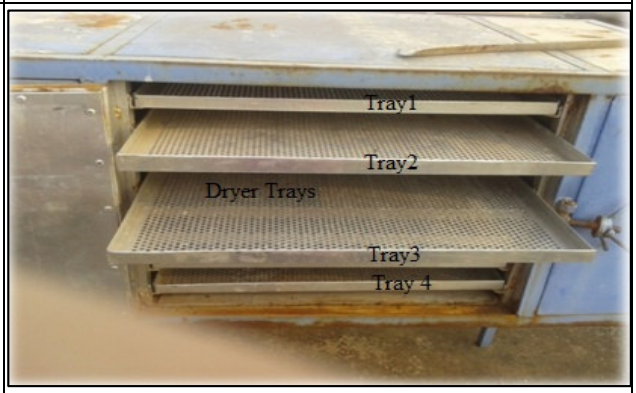

Fig.4.Photograph of the drying chamber

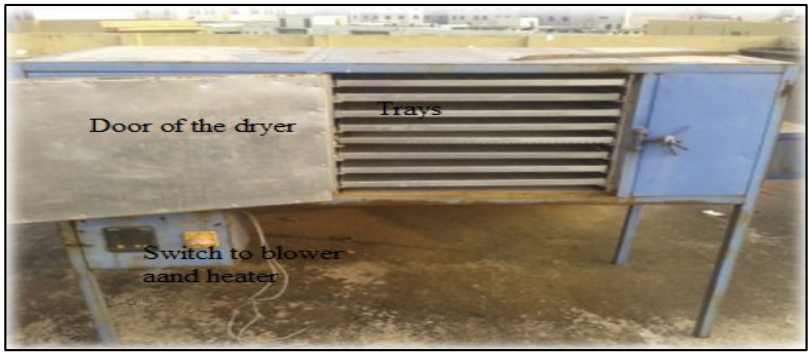

Fig.5.Photograph of the experimental setup

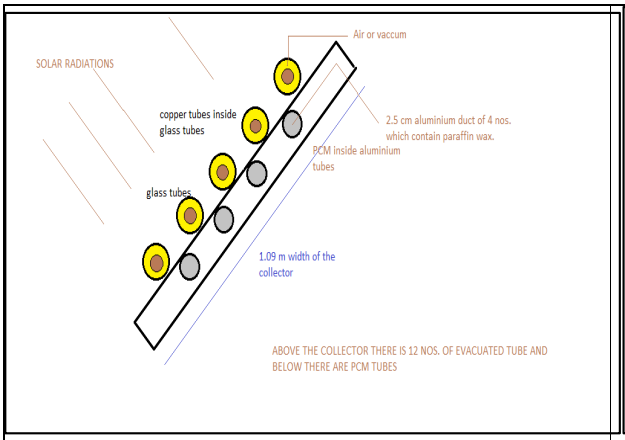

Fig.6. Detailed schematic diagram of the setup with modification.

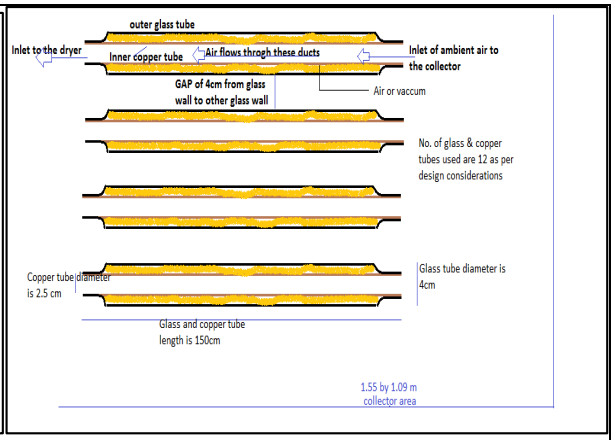

Fig.7.Schematic diagram of the setup with modification (top view).

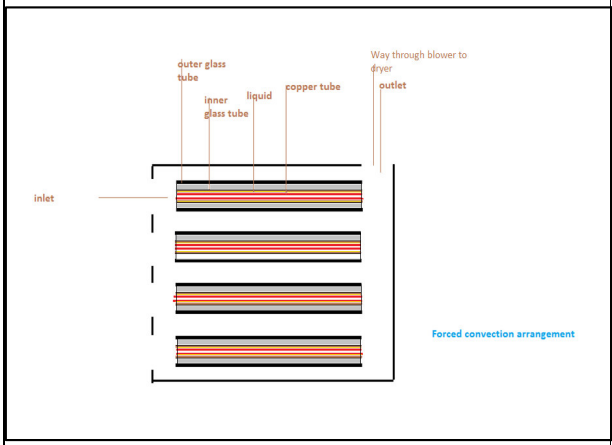

Fig.8.Schematic diagram of the setup with modification

Fig.9.Photographof setup with modification.

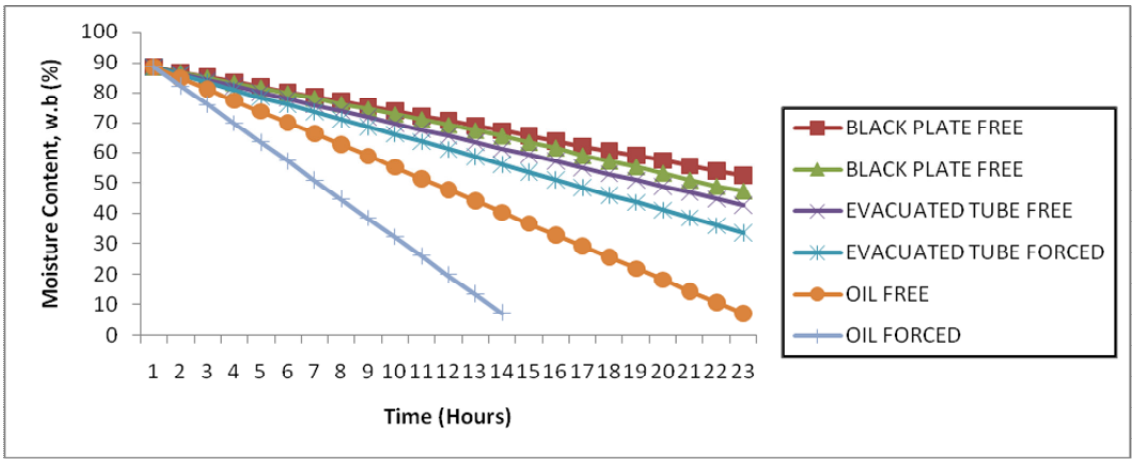

Fig.10.Moisture Content with time for chilli

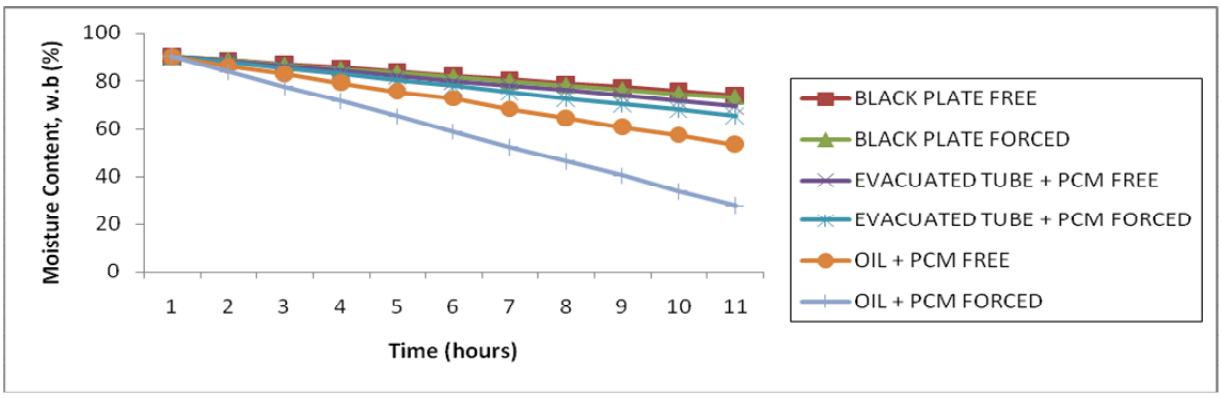

Fig.11.Moisture Content with time for ginger

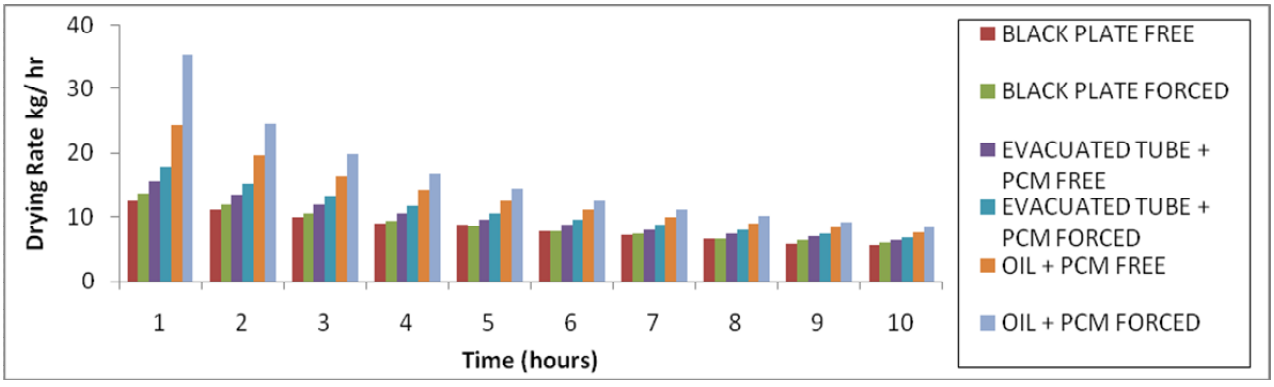

Fig.12.Variation of drying rate with time for chilli

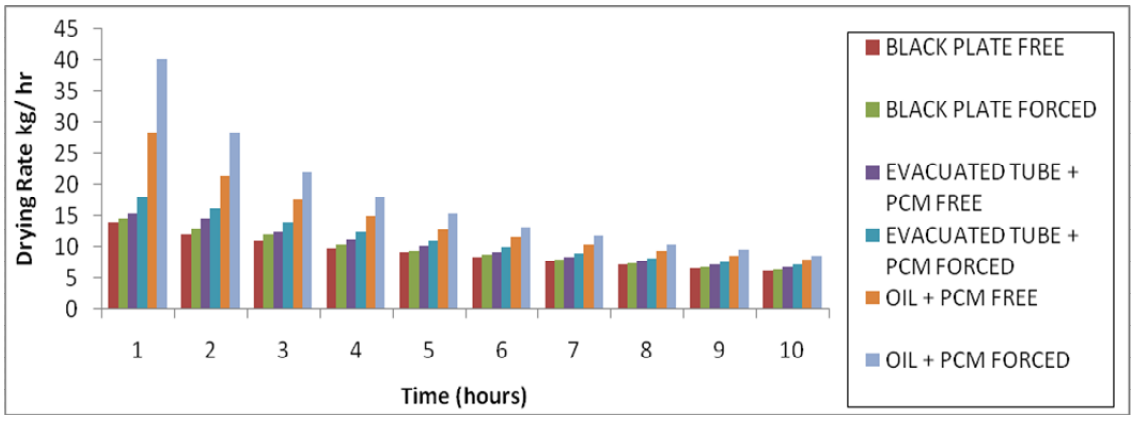

Fig.13.Variation of drying rate with time for ginger

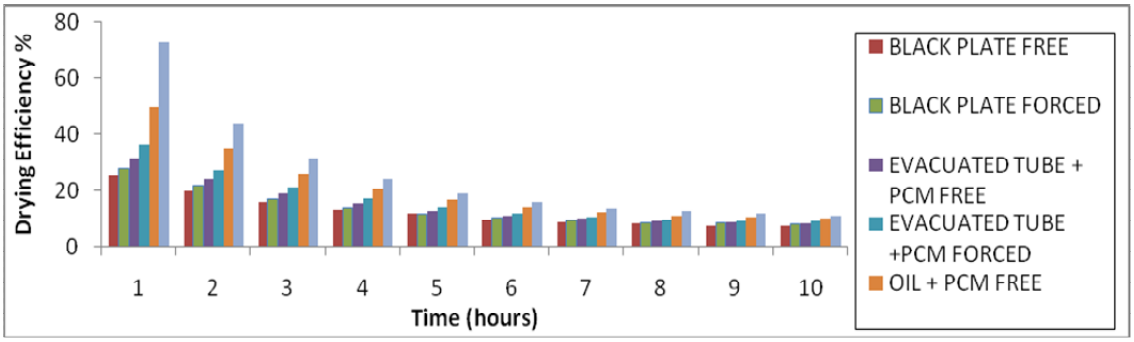

Fig.14.Variation of drying efficiency with time for chilli

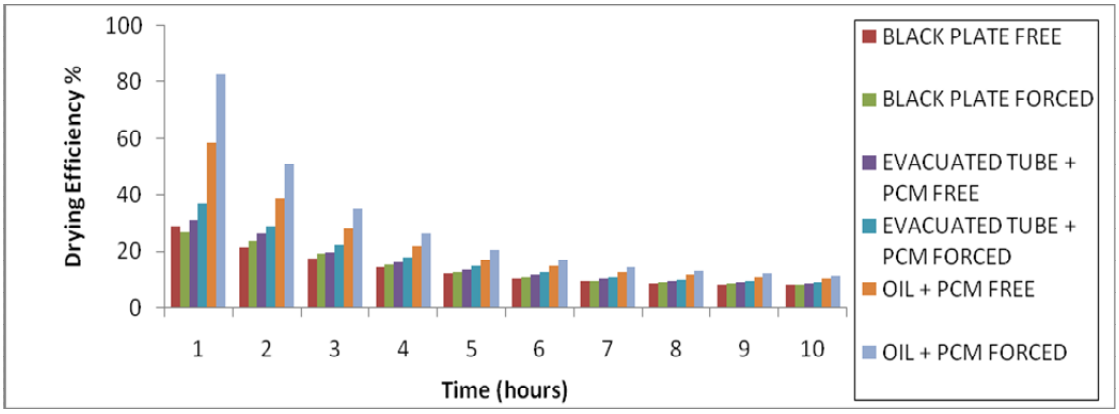

Fig.15.Variation of drying efficiency with time for ginger

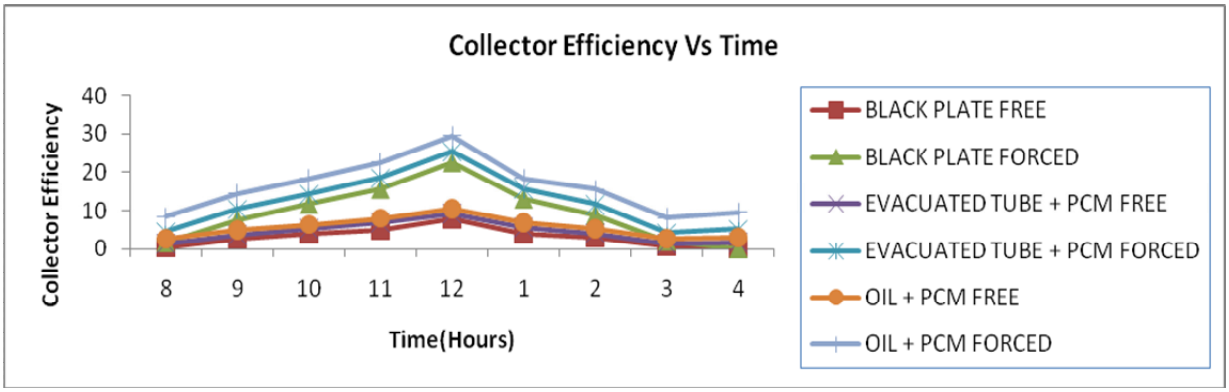

Fig.16.Collector Efficiency with time

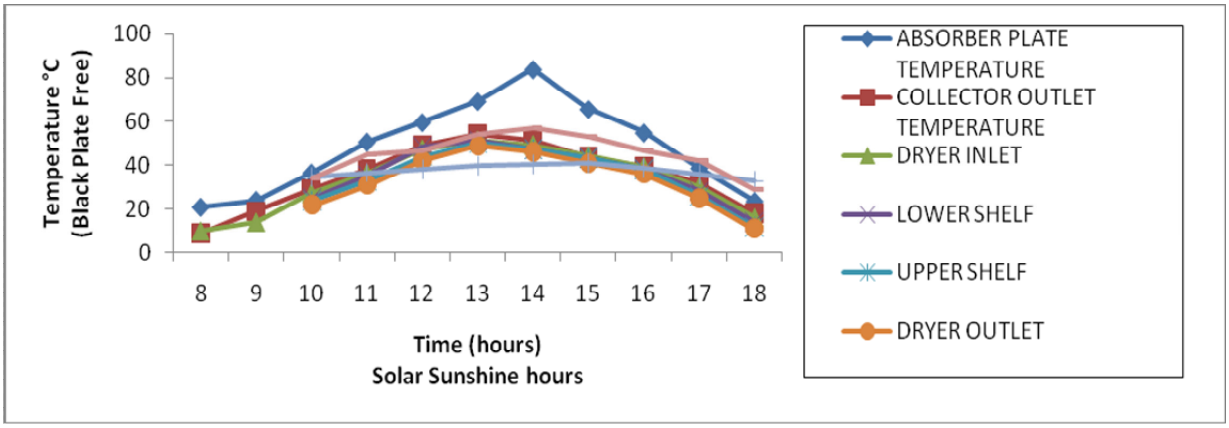

Fig.17.Variation of temperature of black plate in free mode with solar sunshine hours

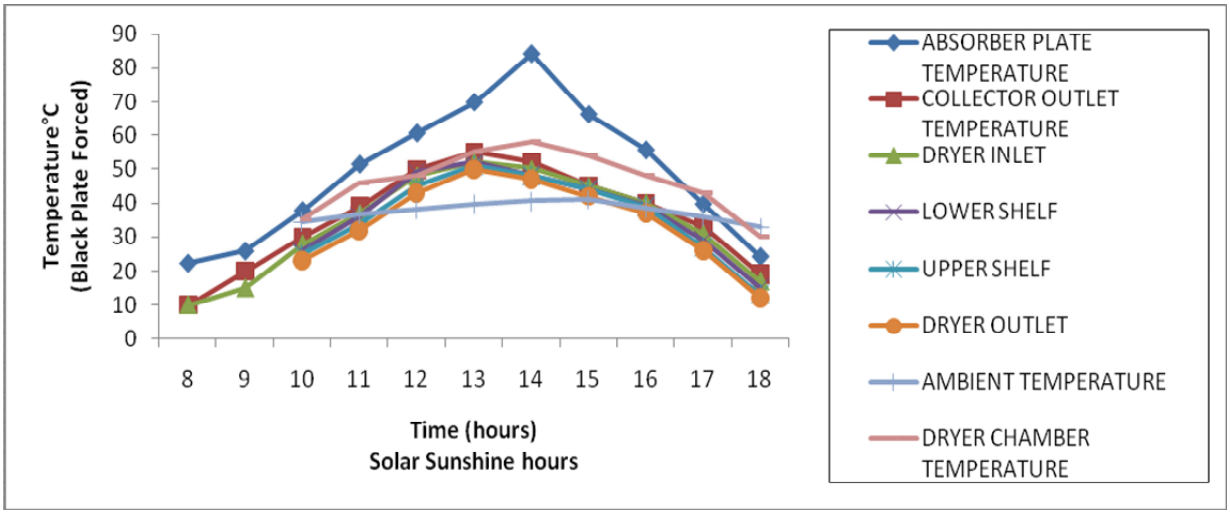

Fig.18.Variation of temperature of black plate in forced mode with solar sunshine hours

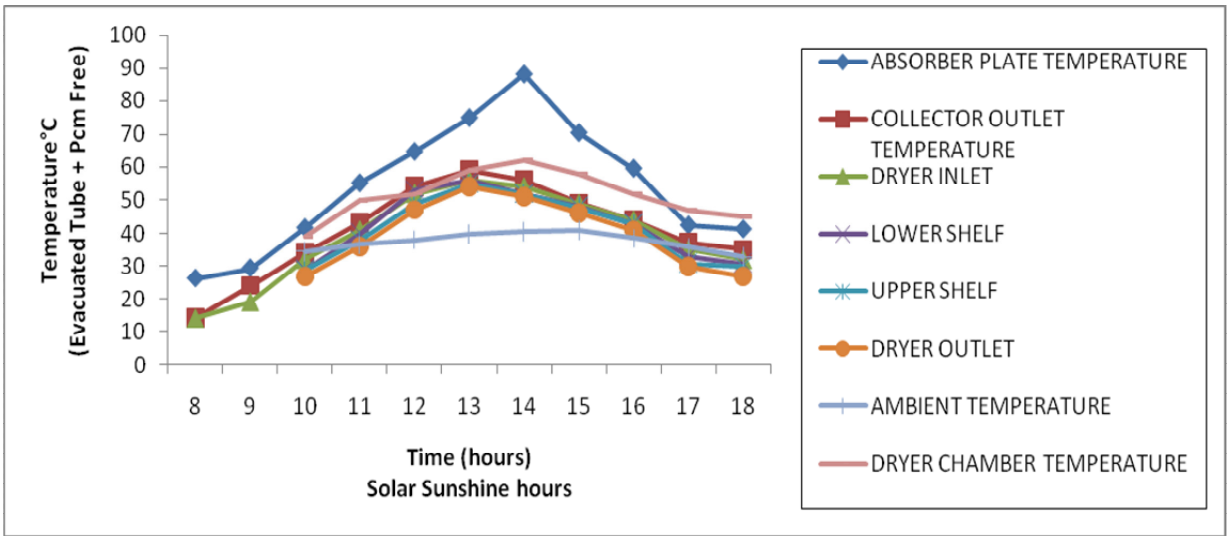

Fig.19.Variation of temperature of evacuated tube with PCM in free mode with solar sunshine hours

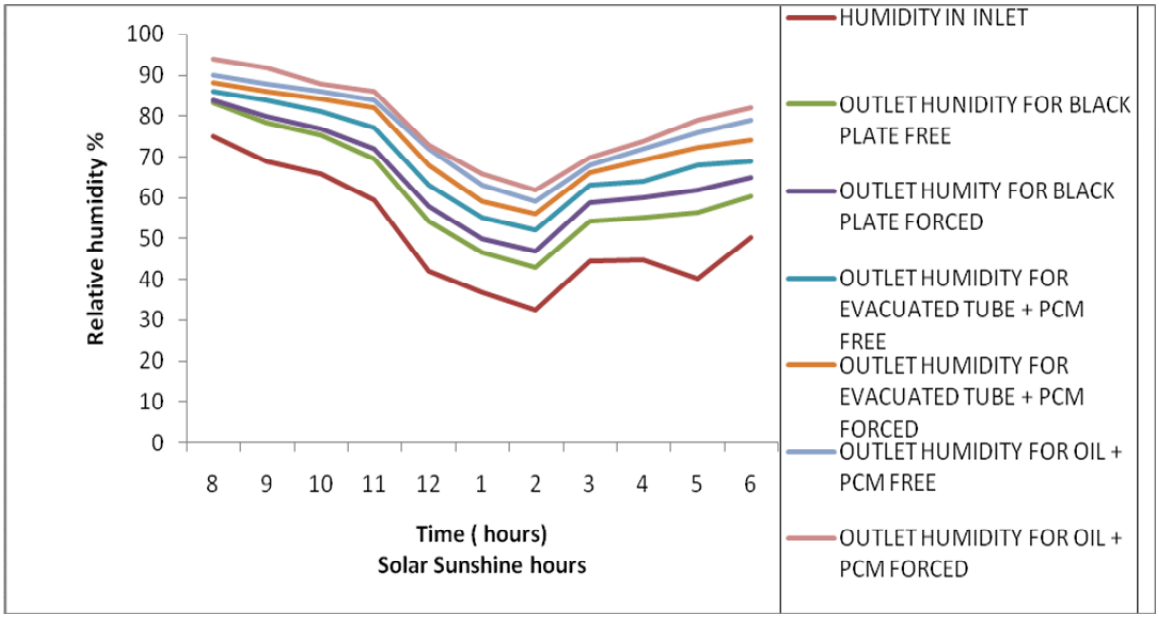

Fig.20.Variation of humidity with solar sunshine hours

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RESEARCH ARTICLE

CFD Simulation of Vertical Axis Wind Turbine

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ABSTRACT

This article deals with the study of wind turbine under natural wind conditions. It shows the variation of various parameters like velocity, pressure and vorticity with normal wind speed. It is important to get the effect of these parameters in the designing of wind turbines. Because, if there will be any defect in the structure then it will be a great trouble during its operation. Also, drag and lift are necessary to check for the aerodynamic performance of the wind turbines.

Keywords: CFD simulation of wind turbine, aerodynamic body of blades, air flow around vertical wind turbine, processes to solve CFD, meshless simulation.

INTRODUCTION

Rezaeiha et al. proposed the accuracy of turbulence models for the vertical wind axis turbines [1]. Oggiano investigated about the NTNU wind turbines and also have compared its effectiveness with experimental results [2]. Arshad et al. proposed a simplified design approach for high speed wind turbines [3]. Giahi et al. investigated about the effects of dimensional scale on wind turbine using CFD [4]. Goh et al. tested savonius wind turbines with a bluff body [5]. Liu et al. investigated about the creation of equilibrium marine atmosphere for off shore wind turbines [6]. Quallen et al. investigated about the floating off shore wind turbine with variable controller arrangement [7]. Wong et al. investigated about the flat plate deflector for a vertical axis wind turbine [8].
Import the CAD file blades.
(a) Importing the CAD file bladesto the software, which is in parametric IGES format.
(b) Graphic View Menu, then choose: Visualisation mode > Mesh
(c) Graphic View Menu and choose: Show geometrical properties). Observe that it has around 7900 polygons

METHODOLOGY

Problem set-up

If the geometry has holes, fluid will leak inside and it will be initialised with the inlet velocity condition as the rest of the fluid but, because it is confined, generates pressure waves inside of the geometry that lead to wrong forces. Furthermore, closed volumes with a small opening will equilibrate the interior pressure to the local static pressure at the hole, leading to wrong overall forces.

Solution technique

Import the geometry

The geometry used in Step 1 will not be used anymore in this tutorial. Now import the geometry files:
Engine settings
(a) Select the 3d Kernel, Single phase external as Flow model and Isothermal in Thermal model.
(b) Leave the default Turbulence settings.
(c) Expand the Advanced Options and switch On the Acoustic analysis.

Material settings keep the default parameters of Gas, which by default correspond to those of air. Note that there is an additional option related to the acoustics analysis: Enable bulk viscosity; switch it on. Set the same vale for the Volume bulk viscosity than that of the dynamic viscosity, namely 1.7894e-05 Pas.

Simulation settings

(a) Set 0.5 metres as target resolution for the wake, tower and blades (Wake resolution; Shape blades: Target resolved scale; Shape-tower: Target resolved scale) (b) Store data with a Frames frequency of 25 Hz and set the Numerical data frequency to Solver time step. This allows to study in the frequency domain with the solver time step frequency but only save the data at a frequency of 25 Hz. (c) Set the Store data > Folder: Wind-Turbine (d) Leave Save averaged fields and Compute markers disabled.The Probes are working in the same way as the Sensors (used in the Tutorial 04 for example). The difference is that the Probes need to be defined before running the calculation to be accessible in the Function Viewer, but then software does not need to refresh every frame to load the data as with the Sensors. Therefore, this allows you to save time for post-processing when you know in advance where to probe, and furthermore the probes can measure the information at the solver time step instead of the frames frequency as for the sensors.

RESULTS AND DISCUSSION

Fig.1 shows the velocity contours of wind turbine; it clearly shows that the velocity is maximum at the blade portion than as compared to its rear portion. The maximum attainable velocity is 6 m/s, and it is sufficient to rotate the turbine blades.Fig. 2 shows the total pressure distribution on the surface of wind turbine blades. The pressure distribution on the frontal area is less, and this shows that the turbine blades are aerodynamic. Therefore, the wind turbine blades are suitable to be operated in normal wind conditions.Fig. 3 shows the vorticity contour of wind turbine, it clearly shows that the vorticity on the nacelle of wind turbine is high and can lead to instability of the wind turbine under normal wind conditions. Therefore, this part needs modification; so, that the vorticity can be reduced. Fig. 4 shows the turbulence intensity contour of wind turbine; it clearly indicates that the rear portion the nacelle is unstable due to high turbulence. This is only due to long rear end of the nacelle of the wind turbine, and it should be modified.

CONCLUSION

Therefore, it can be concluded that before going for the assembly or production of wind turbine; it should be checked whether it is aerodynamic or not. Also, there should not be any turbulence in the air flow past the wind turbine; otherwise it may create problem during the operation of the wind turbine.

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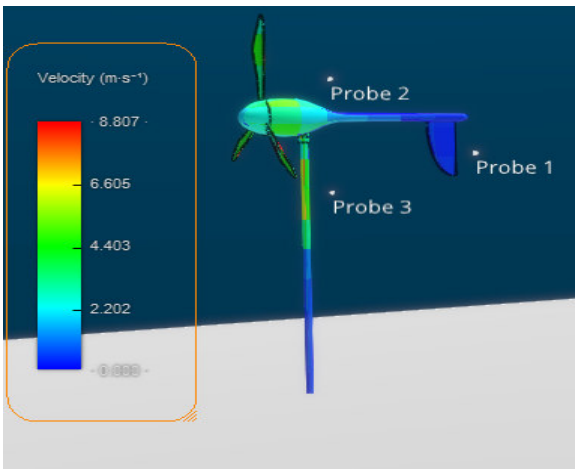

Fig. 1.Velocity contour of wind turbine

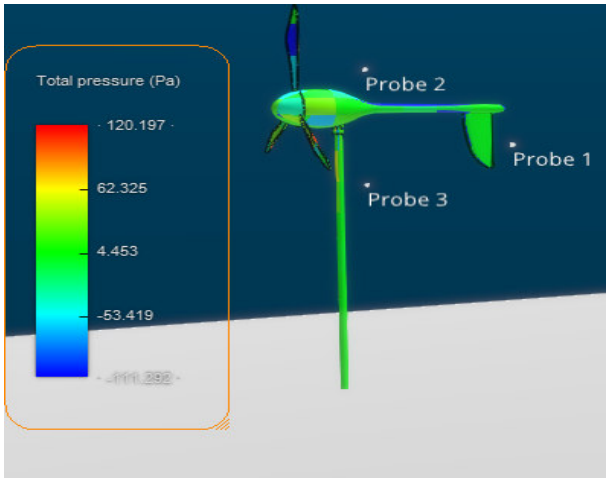

Fig. 2.Pressure contour of wind turbine

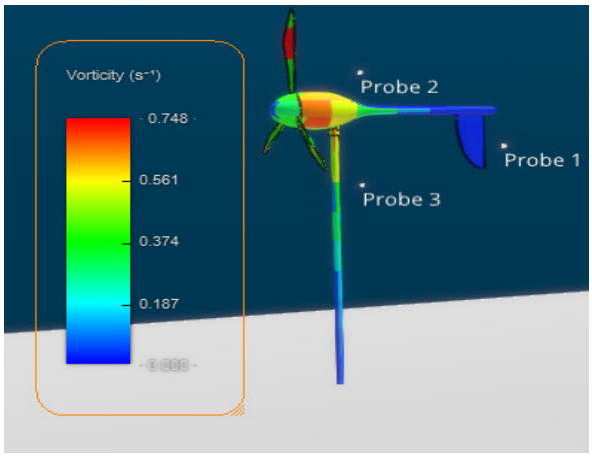

Fig. 3. Vorticity contour of wind turbine

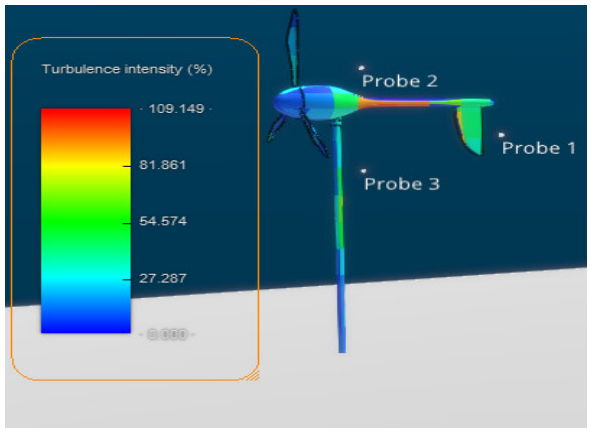

Fig. 4.Turbulence contour of wind turbine.

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REVIEW ARTICLE

The Times of Cyber Attacks

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ABSTRACT

Cyber security's importance is on the rise. Our world relies on technologies more than ever before. Government, military, organizations, financial institutions, universities and other businesses collect, process and store a large amount of information on computers. This trend is growing faster every day. As computers become a major source of information, they need to be protected. Every day a new type of cyber-attack came into an act which makes digital data more vulnerable day by day. Cybersecurity is the practice of ensuring the integrity, confidentiality, and availability (ICA) of information. It requires a broad variety of resources to secure networks, computers, services and data against threats or non-authorized entry, which encompasses best practices for risk control techniques and technologies. In this paper, we will address generations of cyberattacks, attacker strategy, and biggest cyber -attacks in India. The statistical data of cyber-attacks and security will be discussed. The paper will also clarify emerging concepts of information technology and potential protection developments. In this article, intelligent protection strategies will be clarified to secure information from multiple intruders.

Keywords: Confidential data, Cyber-attacks, cybercrimes, Cyber Security, Defense, Hackers

INTRODUCTION

Cyber protection requires technologies, processes and acts to prevent interference, intrusion or unwanted access to networks, equipment, facilities and documents. This involves data storage. It may also be considered protection in the area of information technology. It is important, as states, businesses, and financial institutions and medical organizations gather, process and store data on computers and other tools without precedent. Sensitive details, be it intellectual possession, financial records, personal information or some other records category that could have adverse impacts on unwanted entry or disclosure, may be a major part of this database. The corporation that transmits sensitive data through networks and other instruments in the market sense determines the discipline of

information management, and the processes that are used to administer and retain it. As cyber threats are increasing in scale and scope, businesses and institutions, in particular those responsible for safeguarding public protection, health and financial data, have to take action to secure their confidential details for company and workers. Cybercrime is one of the world's largest and one of the biggest risks to any organization. The impact on society is reflected in the numbers.Cyber protection firms estimate the worldwide expense of cybercrime to $6 trillion by 2021 . This reflects the largest global capital transition in history, threatens opportunities for creativity and production and would be more lucrative than the entire international trade in all big illegal substances. The cost estimates of damage are based on historical statistics of cybercrime including recent year-over-year growth, a dramatic rise in the hostile nation-state and gangs-hacking activities, and a greater cyber-attack surface by 2021. Cybercrimes involve harm, devastation, burglary, stealing of profitability, intellectual property, burglary of personal and financial data, embezzlement, fraud, normal-term post-attack intrusion, forensic analysis, repair and erase hacked and reputational abuse.

India, with over 560 million internet users, ranks just behind China, is the second largest online platform in the world. According to Internet and Mobile Association of India (IAMAI) [1,2], more than 600 million internet users are projected in India by 2021. In 2015 just 17% of Indians were able to use the internet. There were 483 million internet users in India in 2018. In 2023, 666.4 million internet users will be registered, according to the study [3]. It will lift the figure. Because of its untapped potential, India is the world's second largest online sector. The bulk of internet users in India are cell phones internet users who allow the most practical alternatives to the costly hardware that desktops and networks require. As of 2016, India's mobile Internet usage figures is 320.57 million and Indian Internet users estimated 492.68 million by 2022. 390.9 million users were able to navigate the internet via cell phone in 2018. The number will hit 500.9 million internet users in 2023 [3]. This amount is anticipated.

LITERATURE REVIEW

Any significant violation of information security will collapse and destroy the credibility of an entire organization. Cybersecurity risks are not just a problem of major corporations, such as banks, software firms, and state departments, but also the obligation of any other citizen involved with their records. The rate of cyber-crimes is increasing day by day and therefore the analysis of information security statistics and patterns in past years is necessary for us to understand the diabolistic and illegal forms in which data abuses arise and take steps to be secured.

2017

For cybercrimes,2017 was a high year. The number of cyber-safe accidents has almost doubled from 2016 according to the Online Confidence Alliance [4]. This huge spike, from approximately 82,000 accidents in 2016 to approximately 160,000 in 2017, has been credited in the "2017 Cyber Report" [5]. The eye-catching figures of cybercrime in 2017 were further helped by high-profile ransomware attacks like WannaCry and NotPetya. The estimated expense of a violation was $3,62 million in 2017, according to the Ponemon Instituteand IBM's 2017 "Expense of Data Breaching Report" [6]. The most troubling evidence cited in this study were that, with the implementation of public management practices such as patching apps and performing phishing instruction, 93% of accidents may have been stopped. Although 52% of infringements culminated in "real hacking," 15% were induced by lack of safety devices, 11% were triggered by inadequate internal danger control and 8% by phishing, respectively [5].

2018

The biggest DDoS attack ever reported was endured by GitHub [7] in 2018. The assault culminated in 1.3 terabits of GitHub traffic for a second. A team of security experts from Security Research Labs took to the Hack in the Box

security conference to reveal their project: two years in the reverse engineering phase of the operating systems of Android phones, which showed that some handset makers withhold security fixes from users. With fines of up to 20 million [8] or up to 4% of the annual worldwide turnover for those companies caught mishandling user data, GDPR promised to usher in a new age for the processing of personal data.

2019

In 2019, the cyber technology industry grew by 8.7%and the money invested on data management, rules and data privacy law enforcement tools was $124 billion [9,10]. Around 94%of targeted emails use the payload or malware root to add harmful data. 91% of cyber attacks start with a "spear-phishing" text, an increasingly popular type of phishing that allows more precise and personal use of knowledge regarding a target [11]. Billions of dollars of damage is triggered by cybercrimes, as per analysis by Juniper, the figure reached $2 trillion by 2019 [12].

CYBER ATTACK GENERATIONS

The Ist Generation: In the late 1980s, hackers mounted virus attacks on standalone PCs, typically propagated via disks. The affected private users and companies contributed to the creation of anti-virus (AV) products focused on signature info.Examples of first-generation assaults are:

- Elk Cloner (1982): the first computer virus in the world.
- Brain (1986): booting attack.

The IInd Generation: In the mid-1990s, quickly expanding worm attacks emerged straight from the omnipresent Internet, which forced businesses to build a firewall at the infrastructure's periphery to keep the bad people out.Examples of IInd generation attacks include:

- The Morris Worm (1988): One of the first computer worms, leading to the US first felony conviction under the Computer Fraud and Abuse Act.
- Melissa (1999): A mass mailing macro virus.

The IIIrd Generation: During the first years of the new century, criminals began exploiting bugs during software that could impact the businesses exploiting them. That is also about the period when the purpose of the offender switches from appreciation to remuneration. Initially, the botnet was used, particularly for the spam distribution. This attack generation contributes to the creation of IDS systems, which soon incorporated correction capability and became Intrusion prevention systems. Signatures were already based on IDS / IPS.Examples of assaults from the third century include:

- ILOVEYOU (2000): A worm infecting tens of millions of Windows machines.
- SQL Slammer (2003): Denial of service on 75,000 hosts.

The IV Generation: During the early part of the last decade, there were no signs of the emergence in targeted attacks. During a conversation on the absence of clear evidence regarding weapons of mass destruction, citizens were prompted to follow the word "hidden unknowns" invented by then American defence secretary Donald Rumsfeld. Malware application consistency increases and the first rootkit starts to pop up.Types of threats from the fourth generation include:

- Stuxnet (2005-10): State-sponsored development, targeting SCADA systems in critical infrastructure, including the Iranian nuclear program.
- The Target Breach (2013): Not a virus or worm, but a targeted attack on the clothing retailer. The details of 40- 70 million credit cards stolen, 110 million people's personal information breached.
- The DYN Attack (2016): Not a virus or worm, but a massive distributed denial of service (DDOS) attack on the major DNS provider.

The Vth Generation: A wide-ranging mega-attacks funded by the government began in 2017 so that several businesses may execute them. Cybercrime has its internet and escrow networks. There's a busy null-day market. Examples of assaults from the Vth wave are:

- WannaCry (2017): Major ransomware attack affecting 200,000 computers across 150 countries.
- Petya and NotPetya (2016-17): Variance of ransomware used against machines across Europe

BIGGEST CYBER ATTACKS IN INDIA

SIM Swap Fraud

In August 2018, Navi Mumbai arrested two men for cybercrime. They participated in fraudulent practices with regard to the money transfer from the accounts of a variety of people, unlawfully collecting details on the SIM card. This fraudsters obtained details from citizens and prevented the usage of false documents on their SIM cards. They had to transfer four Indian Rupees out of different accounts successfully. We also went to access a few corporations' profiles [13].

Cyber Attack on Cosmos Bank

The Cosmos Bank's Pune branch was targeted in August 2018 by a brazen cyber assault, which saw the loss of almost 94 Crores rupees. By breaching the Cosmos Bank's computer, In Hong Kong, Hackers cleaned out and passed the funds to a trust. The lawsuit was put before Cosmos Bank with a Pune court of cyber assault. Hackers hacked into the bank's ATM network and stole many details from owners of visas and debit cards. The assault did not go against the cohesive banking solution of Cosmos Bank. The deposits and balance sheets remain unchanged and have little impact on the financial statements of the owner. The switching process was built to function as the node of communication between the payment portals and the bank's central banking solution. The malware assault on the switching network created many false alerts that verified many external demands for visas and debit cards. In 28 nations, there were 14,000 sales, more than 450 tickets. 400 cards and 2,800 transactions were used at the state level. This was the first malware assault to break up the link between the payment gateway and the Indian bank [13].

ATM System Hacked in Kolkata

Fraudsters pirated in July 2018 and wiped off almost 20 lakh rupees of different banks' accounts on ATM servers at Canara Branch. More than 50 people were killed and over 300 ATM customers were accused of providing account data in India. Hackers used skimming machine on ATMs to capture debit cardholders' data to execute a minimum purchase of INR 10,000 and an INR cap of 40,000. Two people who collaborated for a foreign group used skimming operations to collect bank data were arrested on 5 August 2018 in New Delhi[13].

Websites Hacked

Between April 2017 and January 2018, more than 22,000 websites have been compromised. The Indian Cyber Emergency Response Team's figures indicate that over 493 pages, including 114 government-owned websites, were compromised with malware spreads. The attacks were to gather information about users on the network infrastructure and device data[13].

FUTURE OF CYBER ATTACKS (Fig.1)

The cybercrime industry has risen with the economic growth of at least $1.5 trillion annually. It is projected to hit $300 billion by 2024 for the cyber-security sector. In 2021, it is estimated that 70% of all purchases for crypto-currencies would be for illicit activity. Cyber-crime costs are estimated at 6 trillion dollars globally by 2021 for corporations and organizations. The loss reported being 20 billion dollars in Ransomware worldwide. An organization's total cybercriminal loss is projected to be 13 million dollars annually [14,15].In the near-decade, there are a variety of big cyber threats. Attacks against IoT would be 34%. A maximum of 98% of IoT computer traffic is authenticated, exposing network data that is sensitive and private. 28% of sensitive infrastructure threats and 20% of devices would be targeted [14]. Using a smartphone and other media, attackers attempted to pass on confidential details to citizens. Such assaults are recognized as virtual infrastructure and will carry 6% of assaults in the future. There are also ongoing advances in cloud infrastructure, which have several bugs that cyber attackers or malicious insiders may use.

DESIGNING FUTURE TECHNOLOGIES WITH SECURITY (Fig.2)

The design of future technologies must provide security. Adding protection afterwards is not enough or viable anymore. Innovation in defence will have more efficient and insightful approaches to face threats. For cooperation and advancement of adoptions, networks and safety requirements must be available. Throughout the design and implementation of their goods, security and protection suppliers must be assured. To avoid compromise and render safety clear to the user, goods and services must be solid. For both parties and systems in the digital world, encryption needs to secure data while it is accessible or used.

SMART SECURITY SOLUTIONS (Fig.3)

Today, all our critical systems are interconnected and computer-driven. The digital and Internet of Things (IoT), Artificial Intelligence (AI) and Big Data and cloud storage etc. would be more relevant to day-to-day tasks and decisions.Such tools have a significant impact on their degree of weakness, relations and complexities.In the future, cyber-attack based technology for Protection and Offensive can be built by organizations. The cybercriminals and hacktivists will try to utilize cyber-technology to transmit their message and raise revenue and violence in the tribunal.To order to contend with cyber threats and to secure records, particular information defence platforms and technology would need to be more mature and more complex. Defence systems need to be linked in such a way that they may function in real-time. Human will not be able to handle all information attacks so in future the dependency on AI will increase. Also, there is a need to cultivate next generation and advanced cyber experts who will know how to drive and develop those systems. We need a stronger protection approach to secure our infrastructure, technologies and knowledge.For now, hacking has become the number one cause of the intrusion, accompanied by ransomware, intruder and outsider agents and unintentional violations. The number of attacks which lead to device failure and data loss continues to grow.Tougher privacy and other legislation related to cybercrime will be implemented to determine and prosecute criminals and avoid cyber-attacks.

This is claimed that what hackers and criminals would be seeking would decide the future of information protection. And it will mostly be the health-related information and also the wealth like credit card and other financial information. For these regions, data defence should then be stronger because the information is the most valuable commodity.The security departments have traditionally been focused on on-site applications but now Azure, cloud with AWS, and SaaS software can be included, causing other critical details to be compromised or breached.Capable computer frameworks must be implemented that can track, identify and handle cyber-attacks and deter them in real-time.

CONCLUSION

The defense of our classified documents, personally identifying details (PIIs), secure health records, financial knowledge, intellectual property, technology and computer networks against intrusion and undermining attempts by offenders and opponents is an essential part in cybersecurity. Cyber threats from every organization's level can arrive.It was becoming really important to warn people about social manipulation schemes like phishing and more sophisticated computer security threats, such as ransomware (such as WannaCry, NotPetya). In this article, we have discussed the drastic increase in the number of internet users in the last few years with the biggest cyber-attacks that took place in India. The generations of various cyber-attacks give us a clear view of how cyber-attacks technologies upgraded from the very beginning.We have also discussed how cyber-attacks will affect us economicallyin the upcoming future and counter technologies to overcome all those cyber-attacks. Smart security solutions are suggested to tackle them.

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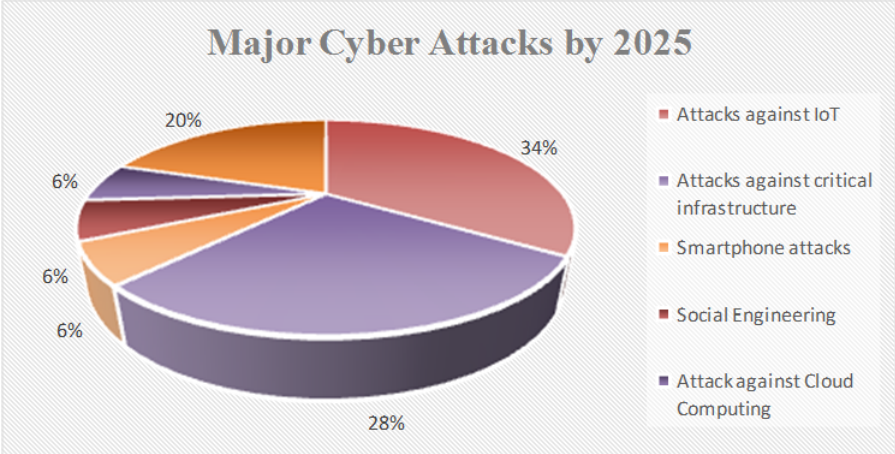

Fig. 1.Major cyber-attacks by 2025

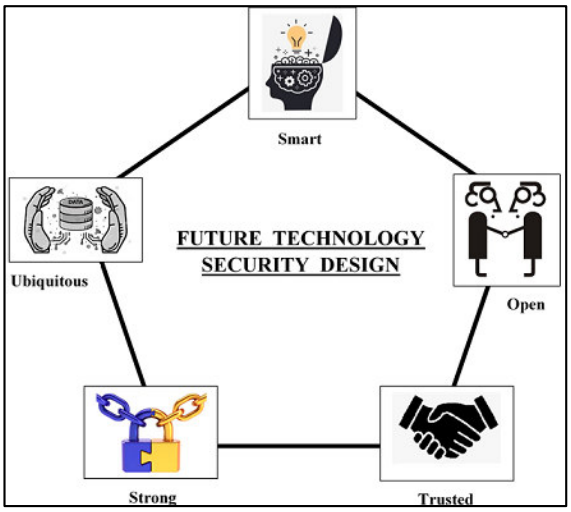

Fig. 2.Future Technology security design

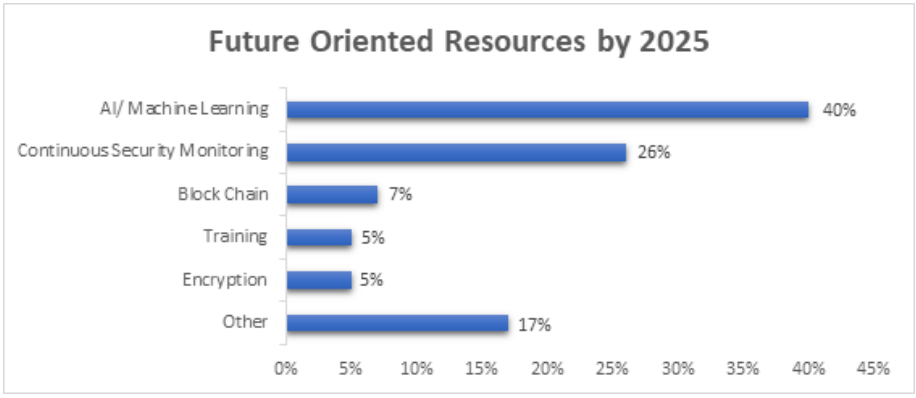

Fig. 3 Resources that are used for security purpose in future [14]

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RESEARCH ARTICLE

Deactivation of 6VXS Enzyme of Corona by Nc1ccc(Nc2ccccc2)cc1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6VXS enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was Nc1ccc(Nc2ccccc2)cc1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [3]. The pharmacophore that was identified had similarity in structure with Apigenin of Passion-flower plant. The important enzyme of corona virus chosen was 6VXS.

RESULTS AND DISCUSSION

Table 1 shows that Apigenin can block 6VXS enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value Nc1ccc(Nc2ccccc2)cc1.

CONCLUSIONS

The results suggested that Apigenin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6VXS enzyme had SMILES value Nc1ccc(Nc2ccccc2)cc1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Apigenin	11.1966	13.2172
2	Pharmacophore	Nc1ccc(Nc2ccccc2)cc1	18.074999999999999	27.549800000000001

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RESEARCH ARTICLE

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Table 1 shows that Apigenin can block 6VXS enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC(=O)[C@H]1SCC(=O)[C@H]1C(=O)OC.

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The results suggested that Apigenin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6VXS enzyme had SMILES value COC(=O)[C@H]1SCC(=O)[C@H]1C(=O)OC.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	COC(=O)[C@H]1SCC(=O)[C@H]1C(=O)OC	19.313700000000001	20.8278

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RESEARCH ARTICLE

Deactivation of 6VXS Enzyme of Corona by OC(=O)C[NH2+]Cc1ccccc1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

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Keywords: Corona, Virus, Docking, Biovia

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Apigenin	11.1966	13.2172
2	Pharmacophore	CCOC(=O)C(=O)N1CCC(CC1) NC(=O)C2CCCCC2	19.5181	35.704599999999999

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RESEARCH ARTICLE

Deactivation of 6VXS Enzyme of Corona by Cn1cnc(C(=O)O)c1C(=O)O

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Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	Cn1cnc(C(=O)O)c1C(=O)O	19.737100000000002	22.321100000000001

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RESEARCH ARTICLE

Deactivation of 6VXS Enzyme of Corona by Cc1cc(C)c(CC(=O)O)c(C)c1

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RESEARCH ARTICLE

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Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	Cc1ccc(O)c(c1)C(=O)NO	20.306999999999999	27.6098

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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Table 1 shows that Apigenin can block 6VXS enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CN(C)C[C@H](O)COCc1occc1.

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The results suggested that Apigenin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6VXS enzyme had SMILES value CN(C)C[C@H](O)COCc1occc1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Apigenin	11.1966	13.2172
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RESEARCH ARTICLE

Deactivation of 6VXS Enzyme of Corona by CCOC(=O)[C@H]1CC[N@@H+](Cc2ccccc2)CC1=O

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6VXS enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CCOC(=O)[C@H]1CC[N@@H+](Cc2ccccc2)CC1=O (SMILES).

Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	CCOC(=O)[C@H]1CC[N@@H+](Cc2ccccc2)CC1=O	21.697199999999999	25.529499999999999

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RESEARCH ARTICLE

Deactivation of 6VXS Enzyme of Corona by C[NH2+]CC(=O)c1ccc(O)c(O)c1

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2	Pharmacophore	C[NH2+]CC(=O)c1ccc(O)c(O)c1	22.4528	23.654399999999999

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RESEARCH ARTICLE

Deactivation of 6VXS Enzyme of Corona by CCOC(=O)CNC(C)(C)C

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RESEARCH ARTICLE

Deactivation of 6VXS enzyme of corona by COC(=O)[C@H](CC(=O)O)C(C)C

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1	Phytochemical	Apigenin	11.1966	13.2172
2	Pharmacophore	COC(=O)[C@H](CC(=O)O)C(C)C	25.151	23.3475

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RESEARCH ARTICLE

Deactivation of 6VXS Enzyme of Corona by Oc1cc([O-])nc2ccccc12

Vinay Dinakaran M* and P Hari Krishna

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RESEARCH ARTICLE

Deactivation of 6VXS Enzyme of Corona by CCOC(=O)C(N(C)C)C(=O)OCC

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

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The results suggested that Apigenin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6VXS enzyme had SMILES value Nc1cc(CCC(=O)O)ccc1O.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Apigenin	11.1966	13.2172
2	Pharmacophore	Nc1cc(CCC(=O)O)ccc1O	27.057700000000001	24.428899999999999

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RESEARCH ARTICLE

Deactivation of 6VXS Enzyme of Corona by CCOC(=O) Cc1c(C)[nH] c2ccc(cc12)C(C)C

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6VXS enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CCOC(=O) Cc1c(C)[nH] c2ccc (cc12) C(C)C (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [3].The pharmacophore that was identified had similarity in structure with Apigenin of Passion-flower plant. The important enzyme of corona virus chosen was 6VXS.

RESULTS AND DISCUSSION

Table 1 shows that Apigenin can block 6VXS enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCOC(=O)Cc1c(C)[nH]c2ccc(cc12)C(C)C.

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The results suggested that Apigenin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6VXS enzyme had SMILES value CCOC(=O)Cc1c(C)[nH]c2ccc(cc12)C(C)C.

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1	Phytochemical	Apigenin	11.1966	13.2172
2	Pharmacophore	CCOC(=O)Cc1c(C)[nH]c2ccc (cc12)C(C)C	29.438099999999999	29.354500000000002

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RESEARCH ARTICLE

Deactivation of 6VXS Enzyme of Corona by [O-]C(=O)C(=O)Cc1ccccc1

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2	Pharmacophore	[O-]C(=O)C(=O)Cc1ccccc1	29.654499999999999	34.474200000000003

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RESEARCH ARTICLE

Deactivation of 6VXS Enzyme of Corona by COC(=O)CS[C@H](C)CC (=O)OC

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Keywords: Corona, Virus, Docking, Biovia

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The results suggested that Apigenin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6VXS enzyme had SMILES value COC(=O)CS[C@H](C)CC(=O)OC.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Apigenin	11.1966	13.2172
2	Pharmacophore	COC(=O)CS[C@H](C)CC(=O)OC	30.994599999999998	33.301000000000002

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RESEARCH ARTICLE

Nitrate-Nitrogen Affects the Fish Productivity in Fish Ponds

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ABSTRACT

Here, we aimed to determine the nitrate-nitrogen ion of the community based ponds in order to validate the suitability of the pond for aquaculture practices. Nitrate-nitrogen ion concentration was measured across three different ponds and finally fish farming was initiated. The nitrate-nitrogen was found to be between 1.76 and 7.95 mg-l^{-1}. This study primarily focuses on making use of unexploited ponds present in the community aiming for introducing fish farming, resulting in an increment in the local economy.

Key words: Community, aquaculture, fish, nitrate-nitrogen, ponds.

INTRODUCTION

With an ever increasing food demand, contribution of fish farming is significant. Water is considered to be a vital natural resource and a critical agricultural input (Huang et al., 2015). Water usage is essential for sustainable agricultural escalation and boost of food availability (Grafton et al., 2015). However, strategies for increasing agricultural productivity need to be focussed. Culture of fish, particularly composite fish culture can be an imperative tool for sustainably recuperating agricultural productivity and for strengthening rural economies (Nagabhatla et al. 2012; Dey and Prein 2006; Dey et al., 2005). Water resources are continuously deteriorating everyday at a quicker rate primarily due to hasty population and urbanization load. Declining water quality is currently a global issue (Mahananda et al., 2010). The water purity varies from place to place in nature (Patil 2013). Essentially, the interaction between physical, chemical and biological components of a habitat determines the quality of water of an ecosystem. Mostly, aquatic biota influences the physico-chemical characteristics of an aquatic ecosystem (Sharma et al., 2009). Limnology essentially deals with inland aquatic ecosystems. Primarily, the growth and survival of fresh water inhabitants depend on the quality of water (Boyd, 1989; Boyd, 1990; Philips, 1991; Jhingran, 1985). Fish plays an important role in agriculture sector of India. It provides livelihood to more than 60 million people and earns more than 6800 crore rupees through export. Extensive limnological studies have been

carried out (Olopade, 2013; Nikolosky, 1963). The quality of water predominantly depends on the physical, chemical and biological characteristics of water (Zweig et al. 1999; Adeniji and Ovie 1982; Das and Padhi, 2014; Padhi et al. 2015). Mostly, the present study is focused on the determination of quality of water in order to utilize the ponds for aquaculture.

MATERIALS AND METHODS

Site of study

For the purpose of study, three ponds (P1, P2 and P3) in three villages in the eastern coastal state of India were chosen for investigation, and such ponds were not utilized for fish cultivation earlier.

Measurement of environmental parameters

The physico-chemical parameter chosen was nitrate-nitrogen ion determination. Measurement was primarily made by following standard procedures (APHA-2005) using water testing kits (NICE), during the period from November 2018 to October 2019.

RESULTS AND DISCUSSION

The maintenance of good water quality is essential for both survival and optimum growth (Gupta and Gupta 2006). The water quality standards vary significantly due to different environmental conditions, ecosystem and intended human users EPA 2006. The quality of aquaculture products and their suitability for human consumption may also be affected by water quality (Zweig et al. 1999). Keeping these factors in view, the ponds under study were maintained for aquaculture imparting training to local people also in order to empower them for gainful employment (Table 1 and Fig.1).

CONCLUSION

During the period of study, care of the ponds was monitored by a group of peer volunteers from each village who have assisted in managerial activity and watch of the ponds in their respective villages. The profit of the sale proceeds of fish was being used as seed money by the volunteers for cultivation of fish for livelihood besides other engagements. Thus the objectives have been achieved through training and interaction sessions generating confidence among the villagers for aquaculture for their livelihood.

Author contribution statement

Sasmita Panda conceived the idea. Pradip Kumar Prusty, Gagan Kumar Panigrahi, Annapurna Sahoo, performed the experiments. Sasmita Panda analyzed the results. All authors contributed significantly in drafting the manuscript.

Funding

The present study was financially supported by Centurion University of Technology and Management, Odisha, India.

ACKNOWLEDGEMENTS

Authors are thankful to the administration and management of Centurion University of Technology and Management, Odisha, India for providing necessary facilities to conduct the experiment.

Conflict of interest

The authors declare that they have no conflict of interest.

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Fig.1: Variations in nitrate-nitrogen (mg-l^{-1}) in different ponds in the study area.

Table I: Variations in nitrate-nitrogen (mg-l^{-1}) in different ponds in the study area

Month-Year	Pond 1 (P1)	Pond 2 (P2)	Pond 3 (P3)
Nov-18	3.2	4.38	10.95
Dec-18	2.56	4.96	8.36
Jan-19	1.26	5.32	7.48
Feb-19	1.26	2.1	2.38
Mar-19	2.15	2.09	2.86
Apr-19	1.35	1.85	5.69
May-19	4.1	4.56	15.35
Jun-19	5.28	3.75	13.92
Jul-19	5.1	8.1	12.89
Aug-19	4.12	5.82	12.4
Sep-19	3.24	6.89	12.96
Oct-19	4.36	7.26	11.1
Nov-19	2.87	6.95	10.42

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RESEARCH ARTICLE

Temperature Adversely Affects the Fish Productivity in Fish Ponds

Pradip Kumar Prusty[1], Gagan Kumar Panigrahi[1], Annapurna Sahoo[2] and Sasmita Panda[3]*

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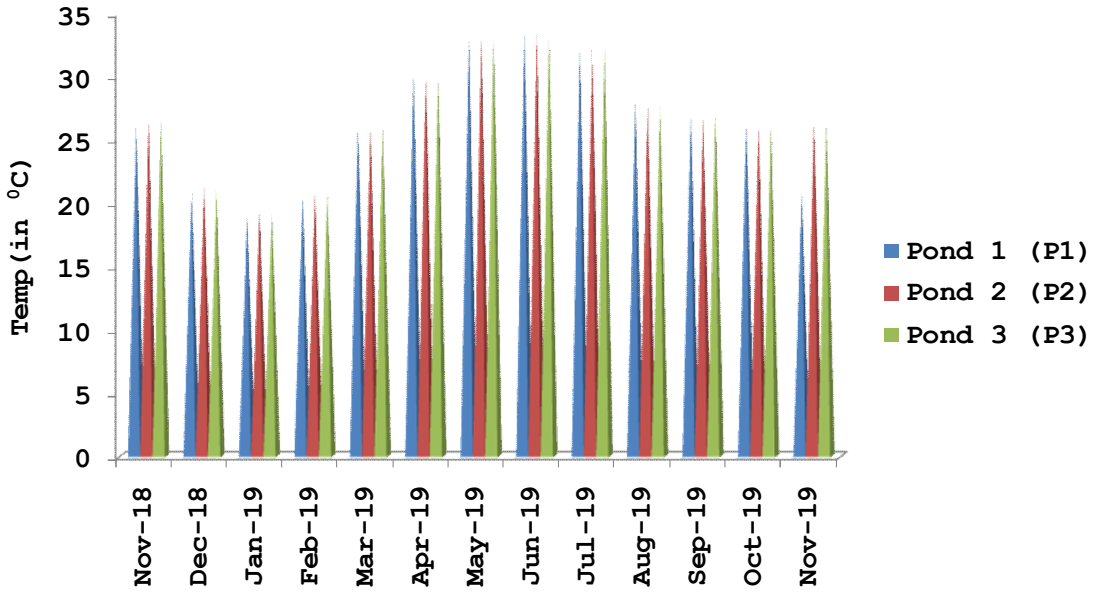

Fig.1: Temp. (in ^{0}C) (Average value) in different ponds in the study area.

Table I: Temp. (in ^{0}C) (Average value) in different ponds in the study area.

Month-Year	Pond 1 (P1)	Pond 2 (P2)	Pond 3 (P3)
Nov-18	26	26.4	26.5
Dec-18	20.8	21.1	21
Jan-19	19	19.3	19.2
Feb-19	20.5	20.8	20.6
Mar-19	26.1	26	26.1
Apr-19	30.2	30	30.1
May-19	33	33.1	33
Jun-19	33.3	33.5	33.1
Jul-19	32	32.1	32.1
Aug-19	28	27.6	27.6
Sep-19	27	26.8	27
Oct-19	26.3	26.1	26.1
Nov-19	20.8	26.5	26.4

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RESEARCH ARTICLE

Ammonia-Nitrogen Affects the Fish Productivity in Fish Ponds

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ABSTRACT

Here, we aimed to determine the ammonia-nitrogen ion of the community based ponds in order to validate the suitability of the pond for aquaculture practices. Ammonia-nitrogen ion concentration was measured across three different ponds and finally fish farming was initiated. The ammonia-nitrogenwas found to be between 1.09 and 12.65 μg-l^{-1}. This study primarily focuses on making use of unexploited ponds present in the community aiming for introducing fish farming, resulting in an increment in the local economy.

Key words: Community, aquaculture, fish, ammonia-nitrogen, ponds.

INTRODUCTION

With an ever increasing food demand, contribution of fish farming is significant. Water is considered to be a vital natural resource and a critical agricultural input (Huang et al., 2015). Water usage is essential for sustainable agricultural escalation and boost of food availability (Grafton et al., 2015). However, strategies for increasing agricultural productivity need to be focussed. Culture of fish, particularly composite fish culture can be an imperative tool for sustainably recuperating agricultural productivity and for strengthening rural economies (Nagabhatla et al. 2012; Dey and Prein 2006; Dey et al., 2005). Water resources are continuously deteriorating everyday at a quicker rate primarily due to hasty population and urbanization load. Declining water quality is currently a global issue (Mahananda et al., 2010). The water purity varies from place to place in nature (Patil 2013). Essentially, the interaction between physical, chemical and biological components of a habitat determines the quality of water of an ecosystem. Mostly, aquatic biota influences the physico-chemical characteristics of an aquatic ecosystem (Sharma et al., 2009). Limnology essentially deals with inland aquatic ecosystems. Primarily, the growth and survival of fresh water inhabitants depend on the quality of water (Boyd, 1989; Boyd, 1990; Philips, 1991; Jhingran, 1985). Fish plays an important role in agriculture sector of India. It provides livelihood to more than 60

million people and earns more than 6800 crore rupees through export. Extensive limnological studies have been carried out (Olopade, 2013; Nikolosky, 1963). The quality of water predominantly depends on the physical, chemical and biological characteristics of water (Zweig et al. 1999; Adeniji and Ovie 1982; Das and Padhi, 2014; Padhi et al. 2015). Mostly, the present study is focused on the determination of quality of water in order to utilize the ponds for aquaculture.

MATERIALS AND METHODS

Site of study

For the purpose of study, three ponds (P1, P2 and P3) in three villages in the eastern coastal state of India were chosen for investigation, and such ponds were not utilized for fish cultivation earlier.

Measurement of environmental parameters

The physico-chemical parameter chosen was ammonia-nitrogen ion determination. Measurement was primarily made by following standard procedures (APHA-2005) using water testing kits (NICE), during the period from November 2018 to October 2019.

RESULTS AND DISCUSSION

The maintenance of good water quality is essential for both survival and optimum growth (Gupta and Gupta 2006). The water quality standards vary significantly due to different environmental conditions, ecosystem and intended human users EPA 2006. The quality of aquaculture products and their suitability for human consumption may also be affected by water quality (Zweig et al. 1999). Keeping these factors in view, the ponds under study were maintained for aquaculture imparting training to local people also in order to empower them for gainful employment (Table 1 and Fig.1).

CONCLUSION

During the period of study, care of the ponds was monitored by a group of peer volunteers from each village who have assisted in managerial activity and watch of the ponds in their respective villages. The profit of the sale proceeds of fish was being used as seed money by the volunteers for cultivation of fish for livelihood besides other engagements. Thus the objectives have been achieved through training and interaction sessions generating confidence among the villagers for aquaculture for their livelihood.

Author contribution statement

Sasmita Panda conceived the idea. Pradip Kumar Prusty, Gagan Kumar Panigrahi, Annapurna Sahoo, performed the experiments. Sasmita Panda analyzed the results. All authors contributed significantly in drafting the manuscript.

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Conflict of interest

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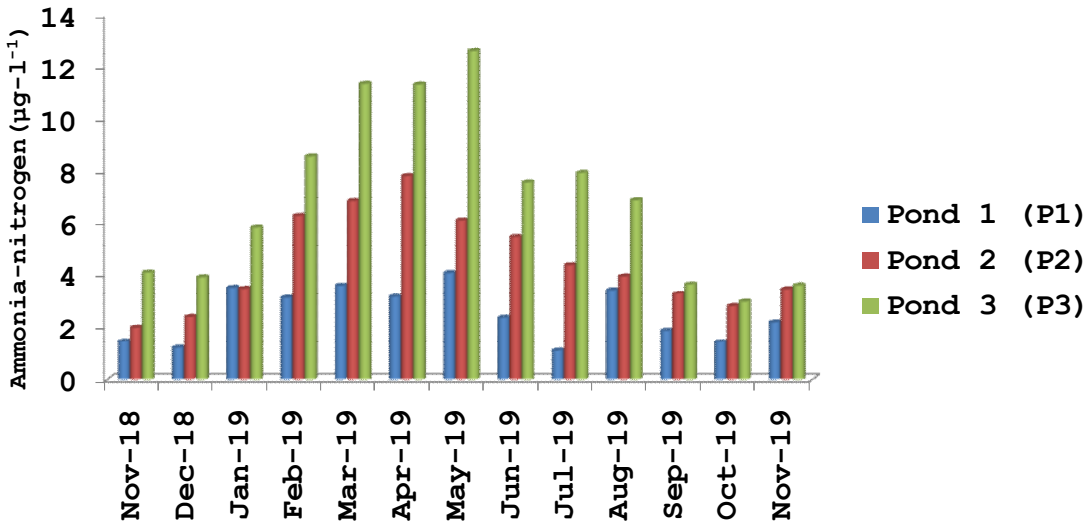

Fig.1: Variations in ammonia-nitrogen (µg-l^{-1}) in different ponds in the study area.

Table I: Variations in ammonia-nitrogen (µg-l^{-1}) in different ponds in the study area.

Month-Year	Pond 1 (P1)	Pond 2 (P2)	Pond 3 (P3)
Nov-18	1.44	1.98	4.1
Dec-18	1.2	2.39	3.92
Jan-19	3.52	3.48	5.84
Feb-19	3.12	6.28	8.56
Mar-19	3.6	6.84	11.38
Apr-19	3.16	7.82	11.35
May-19	4.08	6.1	12.65
Jun-19	2.36	5.48	7.58
Jul-19	1.09	4.38	7.94
Aug-19	3.42	3.95	6.87
Sep-19	1.86	3.28	3.65
Oct-19	1.42	2.8	2.97
Nov-19	2.18	3.46	3.61

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RESEARCH ARTICLE

pH of the Pond Water Affects the Pond Productivity

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ABSTRACT

Here, we aimed to determine the PH of the community based ponds in order to validate the suitability of the pond for aquaculture practices. PH was measured across three different ponds and finally fish farming was initiated. The pH was found to be between 5.4 and 8.3. This study primarily focuses on making use of unexploited ponds present in the community aiming for introducing fish farming, resulting in an increment in the local economy.

Key words: Community, aquaculture, fish, pH, ponds.

INTRODUCTION

With an ever increasing food demand, contribution of fish farming is significant. Water is considered to be a vital natural resource and a critical agricultural input (Huang et al., 2015). Water usage is essential for sustainable agricultural escalation and boost of food availability (Grafton et al., 2015). However, strategies for increasing agricultural productivity need to be focussed. Culture of fish, particularly composite fish culture can be an imperative tool for sustainably recuperating agricultural productivity and for strengthening rural economies (Nagabhatla et al. 2012; Dey and Prein 2006; Dey et al., 2005). Water resources are continuously deteriorating everyday at a quicker rate primarily due to hasty population and urbanization load. Declining water quality is currently a global issue (Mahananda et al., 2010). The water purity varies from place to place in nature (Patil 2013). Essentially, the interaction between physical, chemical and biological components of a habitat determines the quality of water of an ecosystem. Mostly, aquatic biota influences the physico-chemical characteristics of an aquatic ecosystem (Sharma et al., 2009). Limnology essentially deals with inland aquatic ecosystems. Primarily, the growth and survival of fresh water inhabitants depend on the quality of water (Boyd, 1989; Boyd, 1990; Philips, 1991; Jhingran, 1985). Fish plays an important role in agriculture sector of India. It provides livelihood to more than 60 million people and earns more than 6800 crore rupees through export. Extensive limnological studies have been

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MATERIALS AND METHODS

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For the purpose of study, three ponds (P1, P2 and P3) in three villages in the eastern coastal state of India were chosen for investigation, and such ponds were not utilized for fish cultivation earlier.

Measurement of environmental parameters

The physico-chemical parameter chosen was PH determination. Measurement was primarily made by following standard procedures (APHA-2005) using water testing kits (NICE), during the period from November 2018 to October 2019.

RESULTS AND DISCUSSION

The maintenance of good water quality is essential for both survival and optimum growth (Gupta and Gupta 2006). The water quality standards vary significantly due to different environmental conditions, ecosystem and intended human users EPA 2006. The quality of aquaculture products and their suitability for human consumption may also be affected by water quality (Zweig et al. 1999). Keeping these factors in view, the ponds under study were maintained for aquaculture imparting training to local people also in order to empower them for gainful employment (Table 1 and Fig.1).

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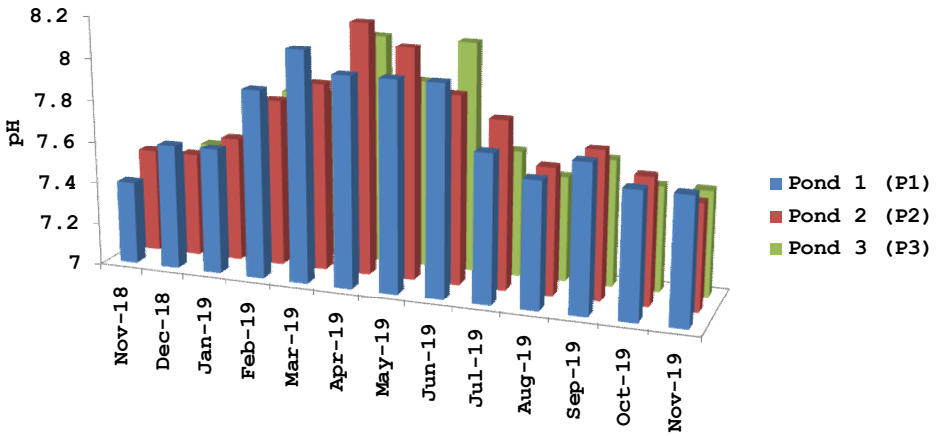

Fig.1: pH (Average value) in different ponds in the study area

Table I: pH (Average value) in different ponds in the study area.

Month-Year	Pond 1 (P1)	Pond 2 (P2)	Pond 3 (P3)
Nov-18	6.8	6.6	6.7
Dec-18	6.5	6.2	6.3
Jan-19	8.5	8	7.9
Feb-19	8.2	8.3	8.1
Mar-19	7.9	7.9	7.8
Apr-19	7.5	7.5	7.6
May-19	5.8	6.1	6.2
Jun-19	5.4	5.5	5.6
Jul-19	5.6	5.7	5.8
Aug-19	7.1	5.7	7.3
Sep-19	7.7	7.8	7.9
Oct-19	7	7.1	7.2
Nov-19	6.7	6.6	6.8

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RESEARCH ARTICLE

Dissolved Oxygen Alters the Fish Productivity in Ponds

Pradip Kumar Prusty[1], Gagan Kumar Panigrahi[1], Annapurna Sahoo[2] and Sasmita Panda[3*]

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ABSTRACT

Here, we aimed to determine the dissolved oxygen of the community based ponds so as to utilize the community ponds for aquaculture practices. Dissolved oxygen was measured across three different ponds of the study site. The dissolved oxygen was found to be between 5.4 and 8.5. This study primarily focuses on making use of unexploited community ponds and ultimately initiating fish farming in the society thereby supplementing the local economy.

Key words: Community, aquaculture, fish, dissolved oxygen, ponds.

INTRODUCTION

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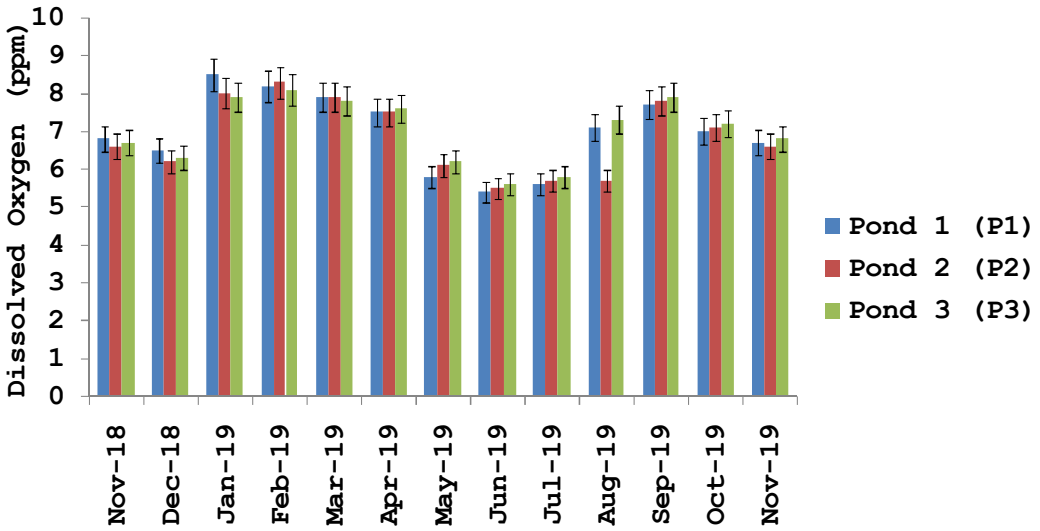

Fig.1: Dissolved Oxygen (in ppm) (Average value) in different ponds in the study area.

Table I: Dissolved Oxygen (in ppm) (Average value) in different ponds in the study area.

Month-Year	Pond 1 (P1)	Pond 2 (P2)	Pond 3 (P3)
Nov-18	6.8	6.6	6.7
Dec-18	6.5	6.2	6.3
Jan-19	8.5	8	7.9
Feb-19	8.2	8.3	8.1
Mar-19	7.9	7.9	7.8
Apr-19	7.5	7.5	7.6
May-19	5.8	6.1	6.2
Jun-19	5.4	5.5	5.6
Jul-19	5.6	5.7	5.8
Aug-19	7.1	5.7	7.3
Sep-19	7.7	7.8	7.9
Oct-19	7	7.1	7.2
Nov-19	6.7	6.6	6.8

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RESEARCH ARTICLE

Comparative Analysis of Monocrystalline and Polycrystalline PV Module using PV-Sol Software

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ABSTRACT

In present day scenario, generation of energy from non-renewable energy has become difficult due to the limited resource of non-renewable energy sources. Therefore researchers are doing research to generate energy from renewable sources in order to meet the energy demand using Solar Photovoltaic module [12]. Different most popular PV solar technologies like Mono crystalline silicon, poly crystalline silicon, amorphous silicon and thin film. The achievement of different type of PV solar technologies depends on the environmental parameters acting upon them. A proper comparison is developed among the mono-crystalline, polycrystalline has been done. PVSolonline software is used to study the characteristics between different types of PV solar technologies.

Keywords : Solar cell; solar irradiation; PV array; temperature; amorphous; crystalline

INTRODUCTION

In present scenario, the generation of electricity from non-renewable sources has become a challenging task. Therefore, in order to overcome the decreasing non-renewable sources, generation of electricity from renewable sources have taken place [1]. The generation of electricity from solar energy is done with the help of PV cells. PV is gives positive attention due to non intervention of thermal process ([4]-[6]). Utilization of solar energy in correct way can help us to meet the increasingdemand of energy ([1],[7-9]).The relationship between voltage and current in case of Photovoltaic solar cell is non-linear and this non-linearity varies with the temperature and solar radiation [1].Different most popular PV solar technologies like Mono crystalline silicon, poly crystalline silicon, amorphous silicon and thin film. [8].For high efficiency, longevity and space efficient monocrystalline PV cells give better result.The disadvantage of monocrystalline PV cell is its high cost [9]. To overcome this disadvantage now a

daysPoly-crystalline solar panels are used. Though the efficiency of this panel is less but still it is popular because of its low cost. The performances of these modules depend on various types of electrical andenvironmental parameters.The entire paper is organised as follows. Section II gives a generalized idea of solar cell. Section III working principle of solar cell and section IV describes the different types of PV cells. Section V gives comparative study of different types of PV cells. section VI. Finally conclusion is drawn at the end.

Solar cell

Solar cells are basically made up of PV system which consists of semi-conducting material responsible for converting the energy of photon into electricity. Whensufficient amount of light strike the panel, photonswith a specific wavelength trigger electrons to flow throughthe materials to produce direct current (DC) electricity([5],[10-14]). To get higher outputvoltage, solar cells are generally connected in series.While for high output current it is connected in parallel structure ([1-4],[11-17]). Incase of PV panel the photovoltaic cells are usually connected in series.

Working of solar cells [11]

A solar cell can be defined as a semiconductor device which helps in conversion of sunlight into electricity with the help of photovoltaic effect [13]. Aphotovoltaic cell is made up of P-type and N-typesemiconductor materials which have different electrical propertiesjoined together [11]. The junction between these twosemiconductors is called P-N junction [11]. The sunlight containsphotonswhen falls solar panel gets absorbed by the semiconducting materials. This result in the creation of electron-hole pairs.Thus, when a solar cell is connected to a load the clectron-hole pair present near the junction separate from each other resulting in collection of holes near the positive terminal and electrons at negative terminal.This helps in creation of electric potential across the terminals. The differencebetween the electric potentials at the terminals result involtage across the terminals [11]. This voltage is used to drive the current in thecircuit. This current in the circuit will be a DC quantity [11]. Atypical diagram of production of electricity from PV panel [11]

Types of PV Cells

A large number of solar cells are present which are made up of different materials. The most common type of solar cells used include Monocrystalline solar cell, Polycrystalline solar cell, Thin film solar cell, Amorphous solar cell, etc. [12] Mono crystalline cells are made up of silicon single crystal which is physically appeared in uniform black shade which indicates high purity of the panel whereas the poly crystalline is made up of multi silicon crystal appeared as different blue shade. Mono cells are octagonal and poly crystalline cells have square shaped cells. These type solarpanels are made by melting raw silicon which is faster andcheaper process than that used for monocrystalline process. Third type of classification is thin film solar cell which ismanufactured by placing one or more films of photovoltaicmaterial (such as Si, Cd, or Cu) on to a substrate sincethese types are easiest to produce and hence these arecheaper. Fourth type of classification is amorphous silicon solar cells (A-Si) which are most widely used in pocket calculators. [11]

CONCLUSION

The comparative study of polycrystalline andmonocrystalline PV module is carried out using PV-sol software. The study shows that, the efficiency of monocrystalline solar panels are typically 15-20% and highest in the market today. Monocrystalline solar panels produce up to four times the amount of electricity as poly crystalline solar panels..

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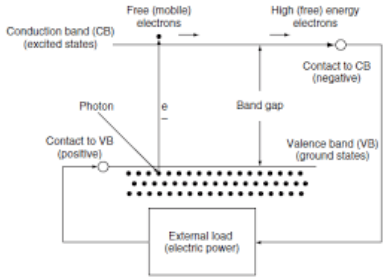

Fig. 2 physics of Solar cell in terms of Band theory

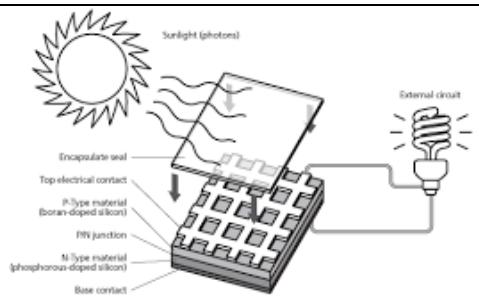

Fig 3. Working of Solar PV Cells

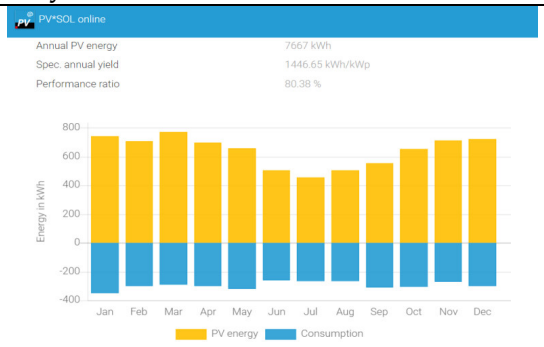

Fig 4. Performance of Monocrystalline PV Module

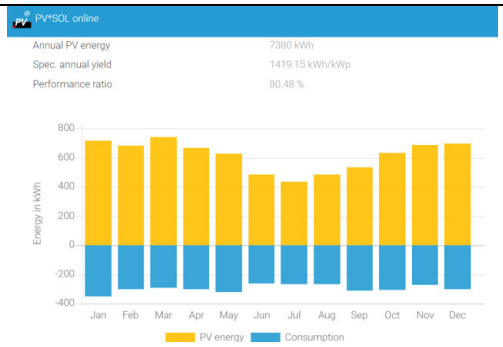

Fig 5 Performance of Polycrystalline PV Module

TABLE 1 : Comparisionbetween monocrystalline and polycrystaline sloar cells

Sl No.	Monocrystalline			Polycrystalline		
	Power Consumption	Efficiency	Solar fraction	Power Consumption	Solar fraction	Efficiency
1	265	16.19	40.9%	260	40.7%	15.89%

A Trina Solar made of up mono crystalline type is selected with 53. KWp.

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RESEARCH ARTICLE

Discrete Behaviour Analysis using Modelica Language Implementation

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ABSTRACT

The framework we have seen is regularly of a simply persistent or discrete nature. The impact of unsettling influence unexpected to the framework altogether perceive by its "discrete conduct" of the framework. In this paper, we'll center around how to communicate what we call "discrete conduct". There is a wide range of building use cases for depicting such conduct and we'll investigate these through the different models introduced in this paper. Ordinarily, when we talk about discrete conduct we regularly allude to "occasions". An occasion is something that happens in our framework that triggers an irregularity. Differential conditions ordinarily bring about consistent arrangements. In any case, when occasions happen, they can present different sorts of discontinuities.

Keywords: Continuous behaviour, Discrete behaviour, Modelica, Object-oriented language, Newton cooling dynamic.

INTRODUCTION

Typically, when we talk about discrete conduct we regularly allude to "occasions". An occasion is something that happens in our framework that triggers intermittence. Differential conditions typically bring about consistent arrangements. In any case, when occasions happen, they can present different sorts of discontinuities. The most straightforward kinds of occasions are ones that occur at a specific time. These are, as anyone might expect, called "time occasions". Since these occasions are attached to the time, we realize what time they will happen even before they occur. Instances of time occasions would be things like changes activated by an advanced clock that is actuated at some predefined recurrence [1]. The other sorts of occasion we will experience are alleged "state occasions". These sorts of occasions are a lot trickier to deal with. The explanation is that we don't have the foggiest idea about from the earlier when these occasions will happen. Not at all like time occasions, have we needed to really hang tight for some

sign in our framework to cross some predefined limit. As a rule, we don't have a clue when that intersection will happen. Besides, deciding the exact second when the occasion happens is to some degree costly [2].In this paper, we'll take a gander at instances of both of these sorts of occasions and the different Modelica language includes that can be utilized to depict when these occasions happen and how we portray reactions to them:

- The conduct to be watched must be a discrete conduct one that has an undeniable start and end.
- It is suggested when conduct happens an extraordinary number of times or if conduct can happen for expanded timeframes.
- Consists of denoting the occasion's objective conduct happens during a predefined timeframe.

Modelica is a general condition based item arranged language for nonstop and discrete-occasion demonstrating of physical frameworks with the end goal of effective reproduction. The language brings together and sums up past article arranged demonstrating dialects [3]. It is achieving an upset around there, in light of its usability, the visual structure of models with a blend of Lego-like predefined model structure hinders, its capacity to characterize model libraries with re-usable segments, and its help for displaying and recreation of complex applications including parts from a few application spaces. In this paper, we present the Modelica language with an accentuation on its language highlights and one of the related re-enactment situations. Recreation models can be created in a coordinated critical thinking condition by utilizing a graphical editorial manager for association outlines. Associations are set up just by drawing lines between objects picked from a class library. The standards of article arranged physical frameworks demonstrating and the multi-area abilities of the language are introduced in the paper by a few models.

COOLING REVISITED

Changing Ambient Conditions

We will begin with a basic model that exhibits time occasions. We will return to the warm model presented beforehand in the segment on Physical Sorts. Nonetheless, this time we will acquaint an unsettling influence with that framework. In particular, we will trigger a sudden decline in the surrounding temperature after a large portion of a moment of reproduction. This updated model is composed as follows: Newton's law of cooling is utilized to display the temperature of an object of some temperature put in a domain of an alternate temperature. The temperature of the article *T(t)* hours subsequent to being put in the new condition is displayed by the equation [4].We will begin with a basic model that exhibits time occasions. We will return to the warm model presented beforehand in the segment on Physical Sorts. Nonetheless, this time we will acquaint an unsettling influence with that framework. In particular, we will trigger a sudden decline in the surrounding temperature after a large portion of a moment of reproduction. This updated model is composed as follows:

Newton's law of cooling is utilized to display the temperature of an object of some temperature put in a domain of an alternate temperature. The temperature of the article *T(t)* hours subsequent to being put in the new condition is displayed by the equation [4].

where:

$$T(t) = T_a + (T_0 - T_a) \cdot e^{-kt},$$

$Ta$is the ambient temperature (the temperature of the surroundings), assumed to be constant and not impacted by the cooling process,T(a) is the temperature of the object after a time of t hours has elapsed, T0 is the initial temperature of the object, and $k$is the decay constant.

```
model NewtonCoolingDynamic
  "Cooling example with fluctuating ambient conditions"
  // Types
  type Temperature=Real(unit="K", min=0);
  type ConvectionCoefficient=Real(unit="W/(m2.K)", min=0);
  type Area=Real(unit="m2", min=0);
  type Mass=Real(unit="kg", min=0);
  type SpecificHeat=Real(unit="J/(K.kg)", min=0);

  // Parameters
  parameter Temperature T0=363.15 "Initial temperature";
  parameter ConvectionCoefficient h=0.7 "Convective cooling coefficient";
  parameter Area A=1.0 "Surface area";
  parameter Mass m=0.1 "Mass of thermal capacitance";
  parameter SpecificHeat c_p=1.2 "Specific heat";

  // Variables
  Temperature T_inf "Ambient temperature";
  Temperature T "Temperature";
initial equation
  T = T0 "Specify initial value for T";
equation
  if time<=0.5 then
    T_inf = 298.15 "Constant temperature when time<=0.5";
  else
    T_inf = 298.15-20*(time-0.5) "Otherwise, decreasing";
  end if;
  m*c_p*der(T) = h*A*(T_inf-T) "Newton's law of cooling";
end NewtonCoolingDynamic;
```

The feature lines show an if proclamation. This specific if explanation gives two distinct conditions to registering T_inf. You will note in this model the variable time isn't proclaimed inside our model. This is on the grounds that time is a worked in factor in all modelica models [5].The choice about which of the two conditions will really be utilized relies upon the contingent expressiontime<=0.5. It is on the grounds that this articulation just relies upon the time and no different factors in our model that we can describe the progress between these two conditions as a "period occasion". The key point is that when incorporating these conditions, we can tell the solver that coordinates our arrangement of conditions to stop accurately at 0.5 seconds and afterward continue again utilizing an alternate condition.

We'll see instances of other state occasions where this would not be conceivable, in the following segment when we present the exemplary Skipping Ball model. Yet, for the time being, let us proceeded with our cooling model. On the off chance that we recreate this model for one second, we get the accompanying temperature direction:

As should be obvious in these outcomes, the encompassing temperature does undoubtedly begin to diminish after a large portion of a second. In examining the dynamic reaction of the temperature itself, we see two particular stages. The main stage is the underlying transient reaction toward balance (to coordinate the surrounding temperature). The subsequent stage is the following of the surrounding temperature as it diminishes [6].

Initial Transients

It is important this is a typical issue in displaying. Much of the time, you wish to show the frameworks reaction to some unsettling influence (like the encompassing temperature decline for this situation). Be that as it may, in the event that you don't begin your framework in a balanced expression, the framework reaction will likewise

incorporate an underlying transient (like the one appeared here). So as to separate these two reactions obviously, we need to evade any cover between them. The most straightforward approach to do that is to begin the recreation in a harmonious condition (as examined past in our conversation of Consistent State Introduction). This keeps away from the underlying transient inside and out and permits us to concentrate altogether on the unsettling influence that we are keen on [7].

As we got the hang of during our conversation of Instatement, we can take care of this issue of beginning drifters by essentially including an underlying condition that will decide an incentive for T with the end goal that our framework begins in a balance state, i.e., The main thing we've changed is the underlying condition. Rather than beginning our framework at some fixed temperature, we start it at a temperature with the end goal that the adjustment in temperature (at any rate at first, preceding our unsettling influence) is zero. Presently the temperature reaction no longer incorporates any underlying transient and we can concentrate just on the reaction to the unsettling influence:

Events

We've seen a few different ways to communicate the way that there is a sudden change in the conduct of our framework. However, it's essential to bring up that we are not simply portraying an adjustment in the surrounding temperature, we are additionally indicating when it changes. This unobtrusive, however significant, point [10][11].

Think about the last model, where our framework started in a harmonious state. Toward the beginning of the recreation, there are no noteworthy elements. Since nothing is truly changing in the framework, the integrator is probably not going to amass critical combination blunder. Along these lines, so as to limit the measure of time required to finish the reenactment, variable time step integrators will, in such conditions, increment their progression size.

```
model NewtonCoolingSteadyThenDynamic
  "Dynamic cooling example with steady state conditions"
  type Temperature=Real(unit="K", min=0);
  type ConvectionCoefficient=Real(unit="W/(m2.K)", min=0);
  type Area=Real(unit="m2", min=0);
  type Mass=Real(unit="kg", min=0);
  type SpecificHeat=Real(unit="J/(K.kg)", min=0);

  parameter ConvectionCoefficient h=0.7 "Convective cooling coefficient";
  parameter Area A=1.0 "Surface area";
  parameter Mass m=0.1 "Mass of thermal capacitance";
  parameter SpecificHeat c_p=1.2 "Specific heat";

  Temperature T_inf "Ambient temperature";
  Temperature T "Temperature";
initial equation
  der(T) = 0 "Steady state initial conditions";
equation
  if time<=0.5 then
    T_inf = 298.15 "Constant temperature when time<=0.5";
  else
    T_inf = 298.15-20*(time-0.5) "Otherwise, decreasing";
  end if;
  m*c_p*der(T) = h*A*(T_inf-T) "Newton's law of cooling";
end NewtonCoolingSteadyThenDynamic;
```

Compactness

One issue with if articulations is that they can roll out moderately basic improvements in conduct show up very confounded. There are two or three elective builds we can use to get a similar conduct with less lines of code [8].

The primary methodology is to utilize an if articulation. Though an if explanation incorporates "branches" containing conditions, an if articulation has branches that contain just articulations. Besides, the sentence structure for an if

articulation is additionally less verbose. In the event that we had decided to utilize an if articulation our condition could have been streamlined to [9]:

```
equation
  T_inf = 298.15 - (if time<0.5 then 0 else 20*(time-0.5));
  m*c_p*der(T) = h*A*(T_inf-T) "Newton's law of cooling";
```

Alternatively, we could use one of the many built-in Modelica functions, like max, to represent the change in the ambient temperature, *e.g.*,

```
equation
  T_inf = 298.15 - max(0, 20*(time-0.5));
  m*c_p*der(T) = h*A*(T_inf-T) "Newton's law of cooling";
```

CONCLUSIONS

This is one of the numerous instances of highlights in Modelica that streamline the manner in which reproduction is done in this paper. An increasing nitty-gritty conversation of this sort of taking care of is appropriately portrayed in this paper. Modelica compilers give the structure of the issue. In this issue, the compiler can see that there is an unmistakable change in conduct. Not just that, it can see that this adjustment in conduct is a period occasion, i.e., an occasion whose time is known from the earlier with no information on the arrangement direction. Along these lines, what a Modelica compiler will do is illuminate the fundamental integrator that there will be an unexpected change in conduct at 0.5 seconds and it will educate the integrator to just incorporate precisely up to that point and no further. Thus, the unexpected change never happens inside a period step. Rather, the integrator will basically restart on the opposite side of the occasion. This totally keeps away from the visually impaired looking for the cutoff time that limits the mistake in the progression. Rather, the integrator will coordinate right up to that point naturally and afterward restart after that point.

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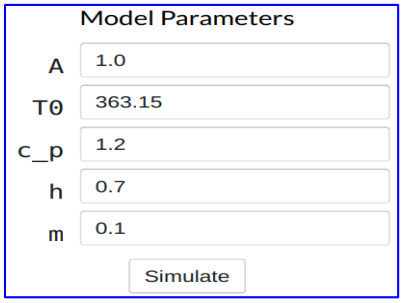

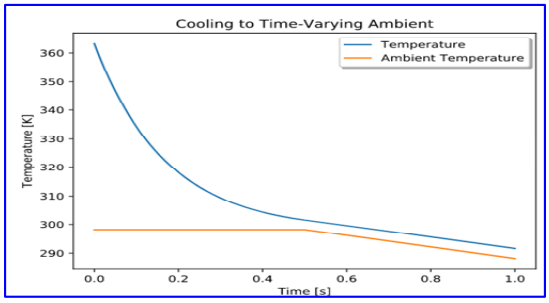

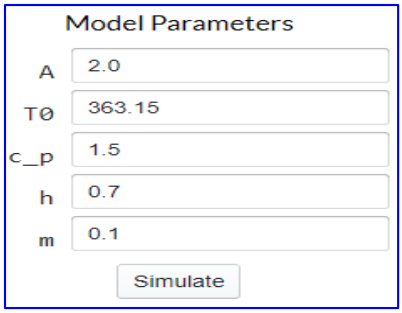

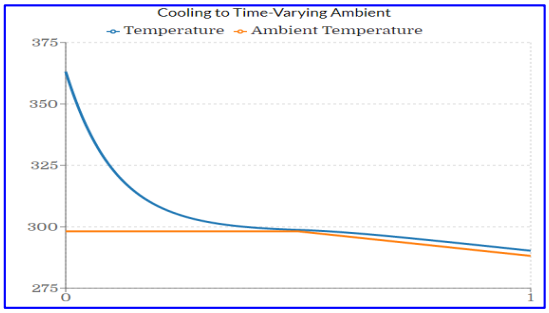

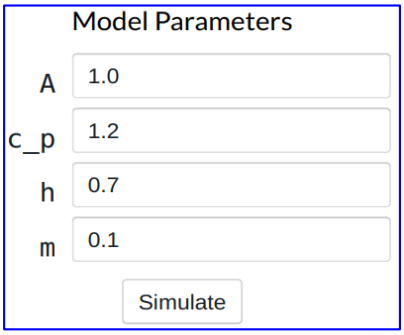

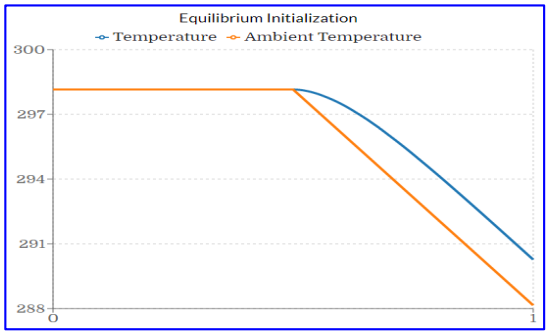

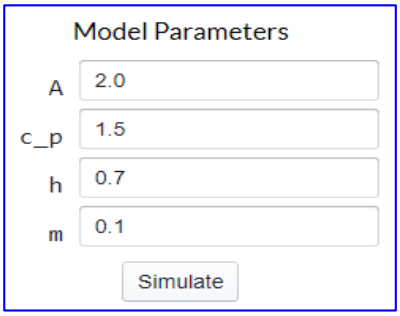

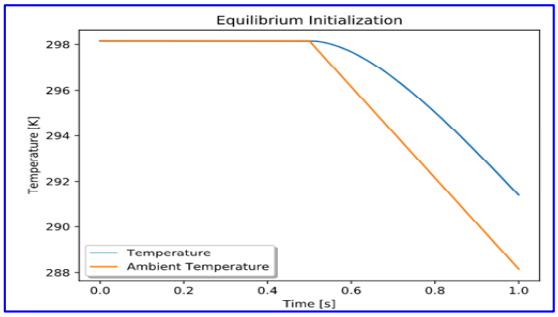

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RESEARCH ARTICLE

Dynamical Modelling for Power Grid using Modelica

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ABSTRACT

Modelica offers the chance of actualizing models of intensity frameworks n an efficient structure. Since Modelica models can be implemented by associating different models, a few pieces of the force framework, (for example, generator power plant models and other control components, and LTC transformers) can be integrated into one smaller model and utilized in grid displaying. Modelica offers the chance of implementing models of power grids in a precise structure.. As the demonstrating technique in reference programming is unique in relation to Modelica, it is important to follow another arrangement of systems.

Keywords: Dymola,Modelica,PowersystemLibrary,PSS,Excite.

INTRODUCTION

It is hypothetically practical to implement and reproduces integral power framework models in Modelica with the vital part models arranged. This paper presents in Modelica [7][9] the encounters of intensity framework displaying [1] and dynamic reproduction. Four structures of fluctuating size are introduced in this investigation. It is hypothetically doable to implement and recreates integral power framework models in Modelica with the important part models arranged. As a rule, various force framework reproduction tests ought to be directed to assess the legitimacy of the picked approach, and the recreation results ought to be approved a couple of endeavors have been made n ongoing years for power framework demonstrating and reenactment utilizing Modelica [5][6].

A few libraries, in any case, are not finished or shut for changes, implying that one can not alter or improve the models. Thus, It is important to build up another force framework library in which so as to direct explicit analyses in the test framework, extra models for the relating gadgets ought to be incorporated into the force framework library. For instance, for voltage soundness tests, the heap tap changer model (LTC) is required. Simultaneously, the models must be numerically precise and have a sensible match with genuine conduct, to accomplish the best reproduction

results. Programming to-programming approval will be done between models dependent on Modelica and the reference programming in which the segments of the force framework were created. To guarantee that the segment models can work well in huge scope framework reenactments, some delegate test frameworks ought to be implemented, and recreation to these test frameworks will be led. The models of the test grid are likewise approved with references. Also, expectation for implement Modelica is to fill in as an answer for the issue of model sharing and co-reproduction between various programming conditions, adjustment and support are conceivable. Such a force framework library is as of now being created at SmarTS Lab inside the setting of the Tesla FP7 venture [8]. Instances of model trade applications are expected to demonstrate the arrangement's achievability.

A)Contribution soft hepaper

1. Give approved models to add to the improvement of the Modelica power framework library.
2. Give approved test framework models to be utilized principally n model approval undertakings, and other powerful security appraisal assignments n the Tesla FP7 venture.

INTRODUCE THE MODEL SYSTEM AN HIERARCHICAL STRATEGY

Modelica provides the ability to apply intensity models in a particular graded way. As models can be implemented in Modelica by interfacing various system models, a few parts of the force system (e.g. generator for power plant im plementations and other control components, and LTC transformers) can be combined into one smaller model and used in frame display.Figure 1 shows a case of a hydroelectric power plant model from Modelica. speed control, Generator, and hydro turbine models are integrated into the hydropower plant model that can be used to demonstrate straightforward in power grid. Since the demonstrating approach n reference programming s not quite the same as Modelica, its important to follow another arrangement of strategies. The means of fruitful displaying are as per the following:

1. Peruse System Specification:If definite segment models are not provided, desired the parts to be accompied as per given application and use in the grid model.
2. Decide the parameters for the models in question. If parameters and information are not determined in the detail, different strategies for identification of parameters (for example identification of estimation based parameters) can be utilized.
3. Model implementation in Modelica.
4. Gather information about the force stream arrangement and initialize the gadget model.
5. Reenactment execution, correlation of recreation results with reference framework. Model.

Nordic 32 KTH Grid

System overview

A form of the purported Nordic 32 test method [10][11] s the principal test framework implemented n this examination, KTH Nordic 32, The framework s anecdotal yet identical to the Swedish and Nordic gridnetwork. KTH Nordic 32 framework single-line graph s indicated n Figure 2. The framework includes 20 generators, 32 transmission and 22 dissemination means of transport, for 74 means of transport n absolute. The test framework s separated into four areas[12][13]:

- North "with some heap and hydro age.
- Central "Equiv" with overwhelming burden and warmth age associated with the North "incorporates a basic outer framework proportionate..
- South "with warm creation, genuinely free to the remainder of the system.

Out of the given test grids 20 generators, 12 are hydro generators found n the North and Equivalent regions, while the rest are warm generators found in the Central and South zone. The framework s intensely accused of huge

exchanges predominantly from north to focal zones, effectively prompting framework instability. The ostensible recurrence would be 50 Hz. Recurrence is constrained by the speed governors at the North and Equiv hydroelectric force plants. G20 s a comparable generator, with a noteworthy involvement n essential recurrence control. This guideline doesn't include the warm units in the Central and South districts. The most extreme force which can be conveyed to the focal burdens is firmly influenced by the Central and a portion of the Northern generators' responsive force capacities. Over-excitation limiters (OELs) impose their receptive force limits. If the force required to be conveyed after an aggravation, (for example, a line blackout) s bigger than the constraints of the generator, voltage instability will result. Initially implemented in PSAT, the KTH Nordic 32 framework is considered the reference for the framework model in Modelica.

Model and data

Transports: The grid has 52 hub means of transport including 20 generator modes of busses. The voltage levels are four: 15 kV for generator busses 20 kV for conveyance busses, 130 kV, 220 kV and 400 kV for transmission busses.

Transmission lines: The grid brags an all-out 52 transmission lines. The model of the transmission line s dependent on the circuit proportionate to π. The qualities are n per unit for opposition r, response x, and susceptance b. Shunt conductance s not considered n this model.

Loads: The grid loads are displayed as steady impedance loads. While initializing the model, with hub voltage greatness U_0, load dynamic force P_0, and responsive force Q_0 are changed from power stream arrangement into steady impedances R_l and X_l:

……..…….(1)

$$P_0 = \frac{R_l U_0^2}{R_l^2 + X_l^2}, \; Q_0 = \frac{X_l U_0^2}{R_l^2 + X_l^2}$$

Shunts:The network has 11 shunts, nine of which are condenser banks and the remainder are inductor banks. The capacitive shunts are positive susceptibility while the inductive shunts are negative eb.

Synchronous generators: The system uses two synchronous generatormodels: three rotor windings for hydro electric plant salient-pole machines (Order V Type 2) and four windings for thermal power plant rotor machines (Order VI). All the data reflects the data proposed by Van Cutsem [14], except for the appar entnominal power of G18, which is modified to1600 MVA. It neglects the effects of saturation.

Turbine governors: The system employs two types of Turbine Governors. For thermal generators TG Type is used while TG Type is used for hydro generators. The data for hydro T Gssgivenin [14], where as for the thermal TGs recommended values are used. The TG Type model is shown Figure 3, and the values for the thermal TGs are used. Form model TGis shown in Figure 3.

Automatic voltage regulators (AVR):For all generators these are used to control the field voltage v_f. Figure 4 shows the AVR model used in type AVR [2] systems. The suggested values are the parameters set out in [15].

Overexcitation limiters: Each generator is fitted with an Over-Excitation Limiter (OEL) to keep with in limitsts field current. Because the focus is on over excited generators, there is no lower limitation to the excitation.The OEL, asseen in Figure 5, is modeled as a purente grator with hard limits to anti-wind up. The OEL will not be triggered unless the current field is greater than t_s flim. The field current is calculated using terminal voltagege nerator v_g, active power p_g, and reactive power q_g. Figure 6 llustrates the system model in Modelica

Simulation and validation

To examine the system's dynamic response, as hort-circuit fault of three phases applied on"Bus 2032"att=15-15:1s,with the fault mpedance Z_{fault} = 0:0001 + j0:001. The fault is set on this bus to decrease then fluence on critical

generators and to avoid affecting the dominant power flow. The validation of the system model is done by comparing Dymola and PSAT response soft wo systems. The machine response is examined after fault by analyzing the following outputs, as shown Figure.7.

- Distribution bus voltage: VB4022, VB2032,VB4012(NORTH)VB1041,VB1043,VB1045VB4041(CENTRAL)
- Generat or terminal voltage:*VG*8,*VG*12(NORTH)*VG*6,*VG*13(CENTRAL)

Generator rotor speed: *w8*(NORTH)*w6*(CENTRAL)

DISCUSSION

As the dissemination transport voltages show n Figure 7, the framework displays damped electro mechanical motions that cease to exist n 10 seconds n reaction to the short out issue applied to one of the generator transport at t = 15s. Since the deficiency s applied to "BUS2032," a non-basic generator transport that s a long way from the North-Central passage, the flaw doesn't influence the predominant force stream. In this manner, the flaw s not making the framework breakdown n voltage. The voltage swaying can be watched n the two territories, for the framework s firmly associated by the 400 kV transmission lines among North and Central regions. Nonetheless, as the flaw s applied to a transport n the north and doesn't result n a significant force misfortune n the focal district, the motions n northern transports are increasingly outrageous. Since AVRs are installed on every generator, the voltage of the terminal s controlled to keep up a steady. The AVRs can be seen running great. Correspondingly, in light of the fact that North Area generators are more influenced than Central Area generators, the voltage motions n G8 and G12 are more serious than G6 and G13.

The G8 (found n North) and G13 (found n Central) generator rotor speeds are kept at around 1 p.u. By ts Governor On generator installed. Also, t can be found from the correlation of the yields from two frameworks That two frameworks react n a pixie comparable design to the unsettling influence. There are minor varieties between the procedures of wavering, the clarification lies n the errors between the two programming numerical solvers

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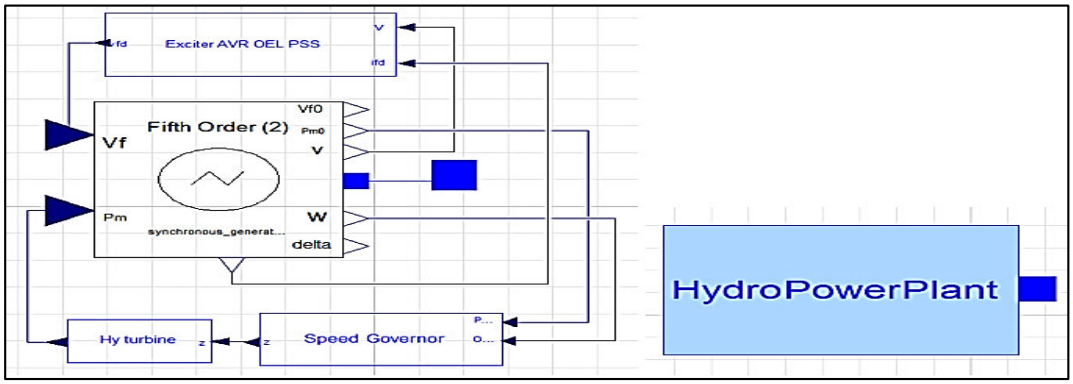

Fig.1.Symbolic and icond is play of model hydro electric power plant in Modelica.

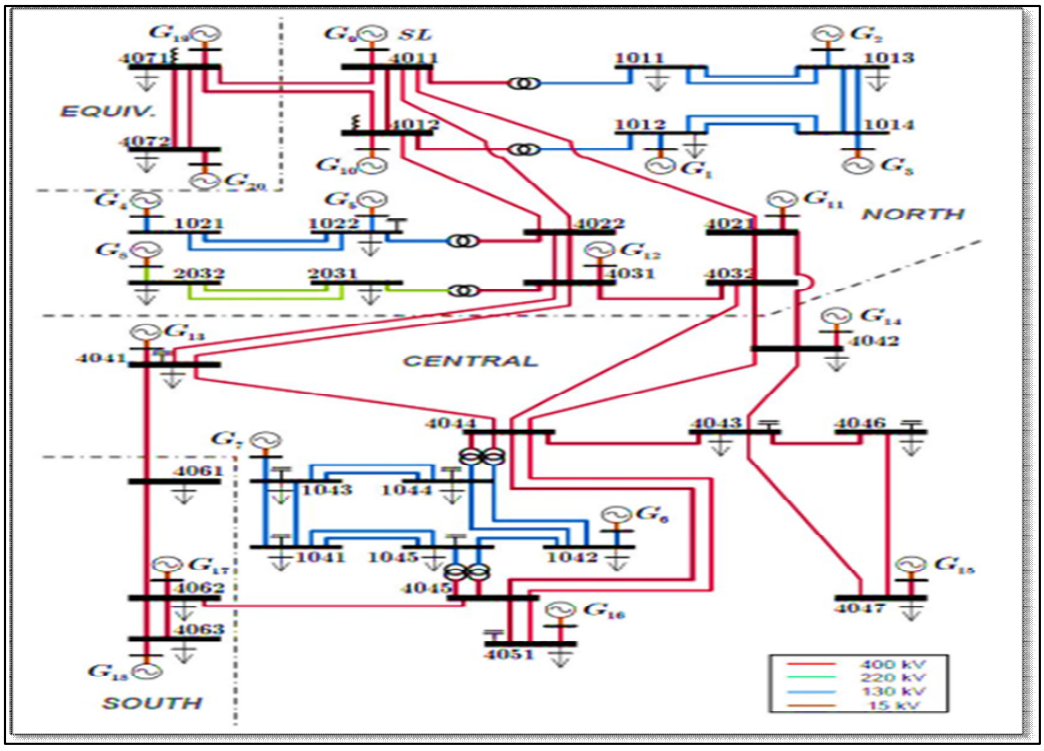

Figure 2: KTHN ordic 32 system [4]

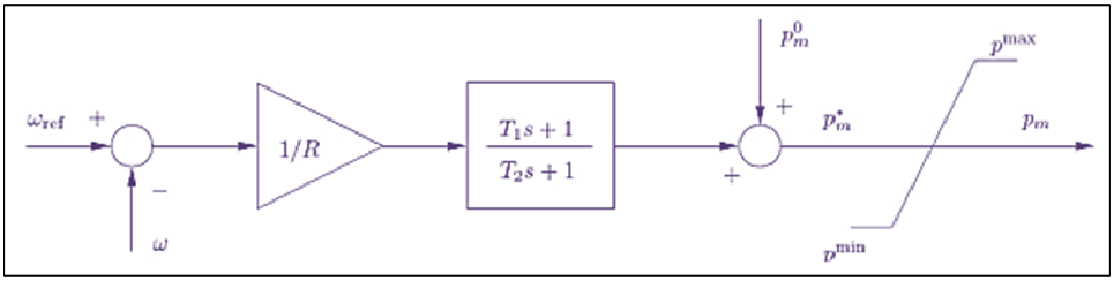

Figure 3: Turbine governor Type model [2]

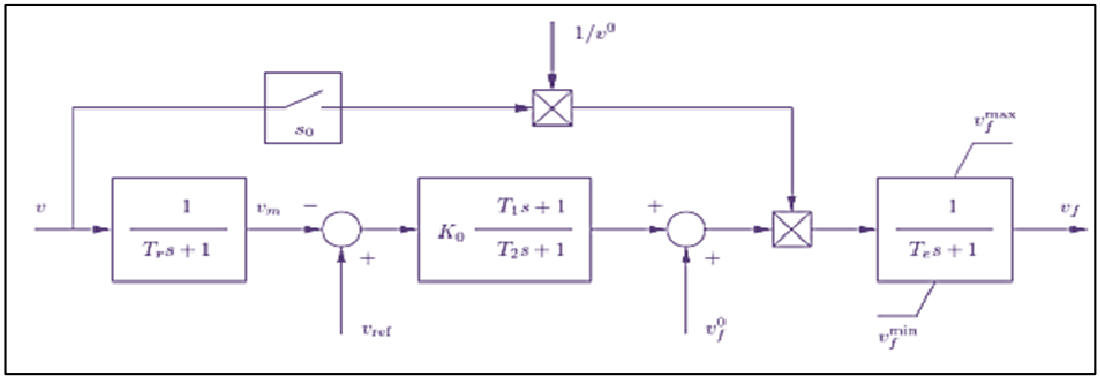

Figure 4: AVR Type model [2]

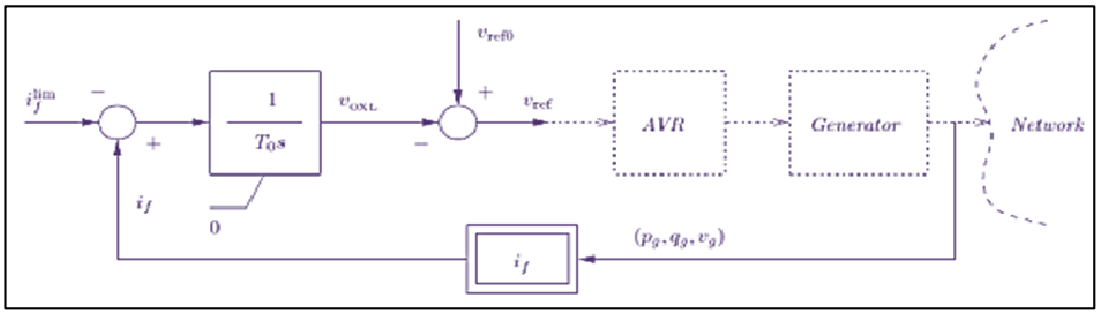

Figure 5: OEL model [2]

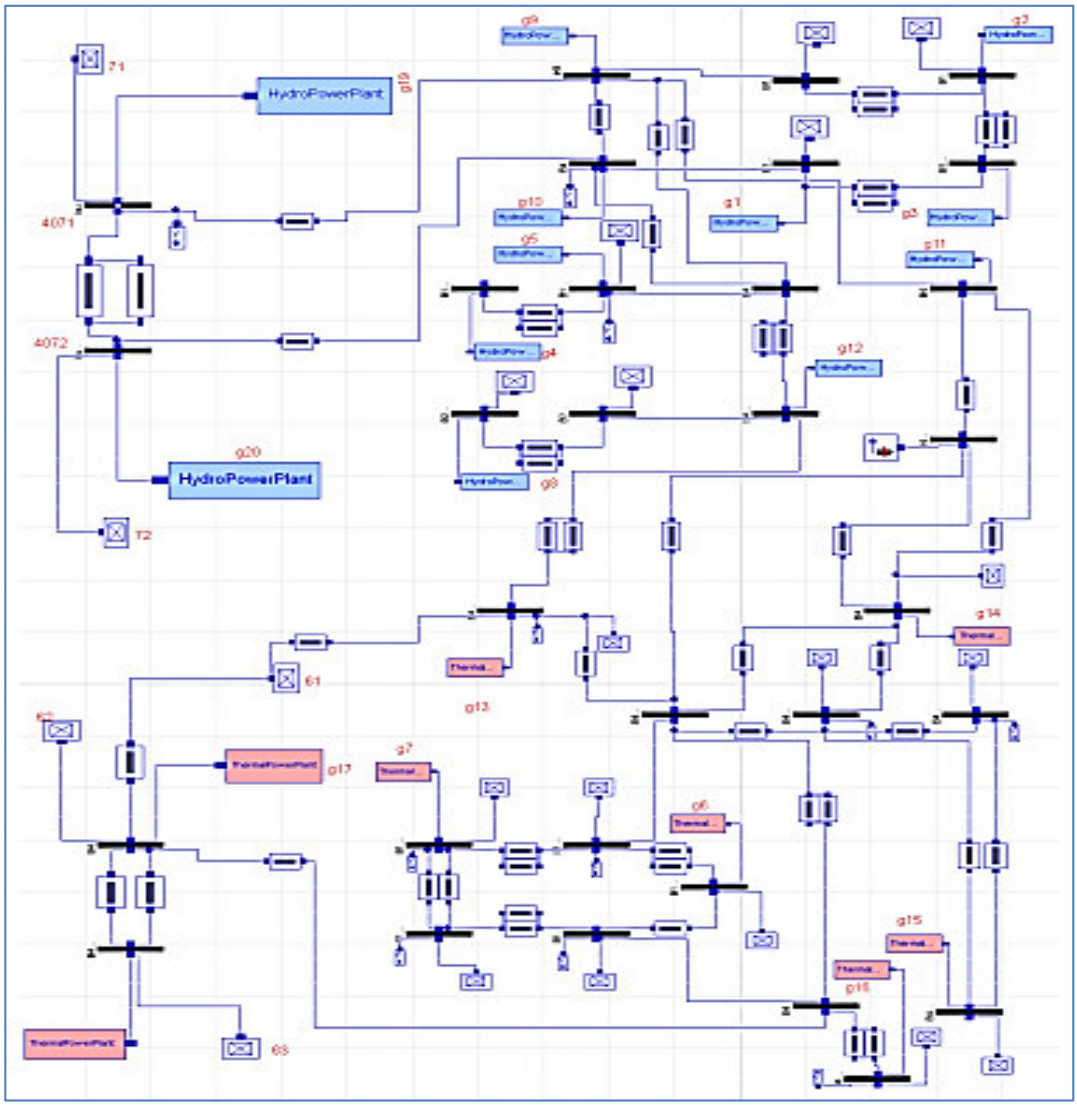

Figure 6: KTH Nordic 32 system model in Modelica

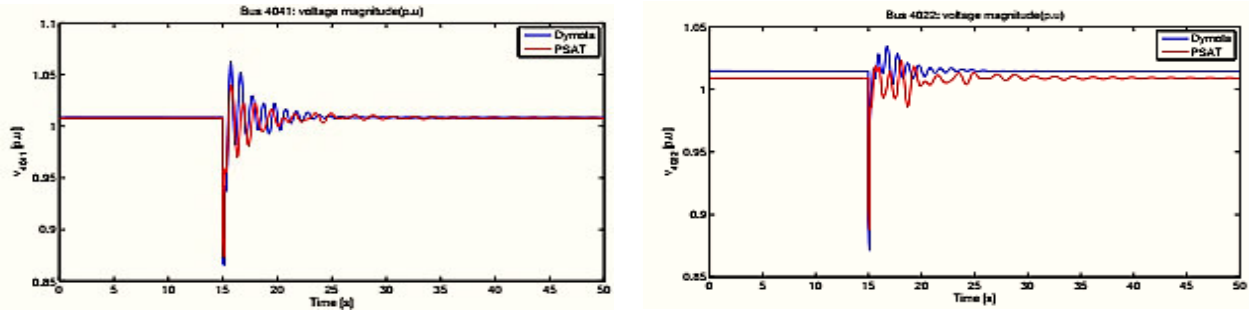

Figure 7: Bus voltages distributed in KTH Nordic 32 system

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RESEARCH ARTICLE

Hybrid Cascaded Modular Multi Level Inverter for a PV Powered Water Pumping System

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ABSTRACT

In order to enhance the quality of voltage or current waveform and to decrease the harmonics content, the level of voltage source inverter is increased to make stair case like waveform and the increased level voltage source inverter is known as multilevel inverter (MLI). A Hybrid Cascaded Modular (HCM) multilevel inverter topology reduces the number of power switches, losses, installation area, voltage stress and converter cost in comparison with the conventional MLIs such as Diode clamped MLI, Flying Capacitor MLI and Cascaded H-bridge MLI. Hybrid cascaded modular MLI uses Nearest Level Control (NLC) modulation technique, which is a low switching frequency modulation technique to generate the gating pulses for the power semiconductor switches. So this HCM MLI with NLC technique becomes an efficient photovoltaic (PV) inverter. It takes the DC power from the PV array through DC-DC boost converter and gives to the induction motor based water pump. In order to maximize the power output and increase the efficiency of a PV module under varying operating conditions, MPPT control is used. MPPT block changes the duty ratio continuously under varying irradiance to keep the output voltage constant. The water pump takes the water form reservoir and stores it into the tank with a constant flow rate and under constant pressure during sunny day and the stored water can be used for domestic applications or any irrigation purposes when the solar irradiance is not available. This type of PV powered pumping system is often suitable for rural areas where the accessibility of grid is not available. It employs Simulink to model a hybrid cascaded modular MLI, DC-DC boost converter MATLAB embedded code to implement perturb and observe (P&O) MPPT algorithm.

Keywords : MPPT, HCM, NLC,TTL, NLC

INTRODUCTION

The sun is a non-polluting resource responsible for the sustained life on earth and can give us efficient renewable energy. The fact that solar energy is cleaner than any other energy produced from fossil fuels makes this resource of sustainable energy very important for the planet future. Generally around 92% of rural population [18] have no access to electricity due to the prohibitive cost of extending the existing electrical network therefore farmers face problems during their cultivation work such as water pumping etc. So the use of renewable energy like photovoltaic (PV) is one the solution for this problem. Therefore PV panel is interfaced with induction motor drive for pumping application via conventional MLI such as diode clamped MLI, flying capacitor MLI and cascade H-bridge MLI etc. But the efficiency of such PV inverter is low and the cost of the PV inverter is more because conventional MLI requires more number of switching devices. In this thesis hybrid cascaded modular (HCM) MLI is taken as PV inverter. To improve the efficiency of PV module we have to use maximum power point tracker (MPPT) [10]. The comparison between PV powered water pumping system Vs. diesel (or Gas) powered system [13] is given in the table. Configuration of a solar PV powered pumping system is shown in the figure 1. All these sections such as PV array, MPPT algorithm, DC-DC boost converter, hybrid cascaded modular (HCM) MLI and Water Pumping system are modelled using MATLAB Simulink.

Proposed System for PV Water Pumping

This thesis proposes a new PV inverter i.e. hybrid cascaded modular (HCM) multi-level inverter (MLI) which is used as an interfacing converter in PV power based pumping system. Figure 2.1 presents the proposed PV system. This includes a PV panel, a boost converter, a three phase HCM MLI nearest level control (NLC) controlled inverter, and a three phase induction motor. An MPPT block is also incorporated into the system so that the input voltage at the converter side can be kept constant.

This proposed system can be categorised into three sub system namely photovoltaic (PV) generator system, inverter unit and the load unit. In photovoltaic (PV) generator system consists of PV array, maximum power point tracker (MPPT) and DC-DC boost converter. In inverter unit, hybrid cascaded modular (HCM) multilevel inverter is used. The nearest level control (NLC) modulation technique is used for generation of gate pulses for the switches of the HCM MLI. The load unit is the induction motor based water pumping system.

The conventional PV water pumping systems consists of a battery backup alongside the components mentioned in the previous section. By incorporating a battery into the system will reduce the lifetime and will also increase the initial cost as well as the yearly maintenance cost of the entire system. With an aim of reducing the overall cost of the system and to increase the lifetime, a new design has been proposed here. The design of this system is done from the load side, taking into account the quantity of water to be pumped and the head at which it has to be stored. So the proposed PV power based water pumping system is the system without batteries unit.

Multilevel Inverter

The term multilevel began with the three level converters. Subsequently, several multilevel converter topologies have been developed. A multilevel converter has several advantages over a conventional two-level converter that uses high switching frequency pulse width modulation (PWM).

There are basically three types of multilevel inverters such as

Diode clamped multilevel inverter (Neutral Point Clamped inverter)

- Diode clamped multilevel inverter (Neutral Point Clamped inverter)
- Flying Capacitor Multilevel Inverter (Capacitor Clamped Inverter)
- Cascaded H-bridge Multilevel Inverter

Apart from these three conventional MLI there is a popular and efficient MLI called hybrid cascaded modular (HCM) MLI. The advantages of the HCM MLI are given below 1. For a given voltage level it requires less number of switches than the conventional one, which in turn results in reduction of installation area and converter cost

Less switching losses because it uses nearest level control (NLC) technique in its modulation technique to provide the gate pulse to switches.

For example in case of a 9-level multilevel inverter, each conventional MLI such as diode clamped MLI, flying capacitor MLI and cascade H-bridge MLI requires 2*(9-1)=16 switches.

Whereas hybrid cascaded modular (HCM) MLI requires only 8 switches for 9-level. Therefore it can be an efficient photovoltaic (PV) inverter for various applications. And to increase overall efficiency of the system hybrid cascaded modular MLI will be incorporated with the photovoltaic (PV) panel to drive induction motor

Modulation Technique

Here we have used tThe nearest level control (NLC) modulation technique to control the output voltage of the hybrid cascaded modular (HCM) multilevel inverter (MLI).Mainly modulation technique can be classified into two types depending upon the switching frequency such as high frequency modulation and low frequency modulation

The Nearest level control (NLC) is low switching frequency control technique. This method is also called as round method. Usually this NLC method is used to provide gate pulse to switches of HCM MLI. This methods leads to reduction in switching losses. The output voltage can be found out by considering a reference sine wave in accordance with nearest voltage level (v). Given a voltage reference vref , the nearest output Voltage level (v) can be determined with

$$v = V * round\{Vref/V_C\}$$

Where, v is the nearest voltage level V is the supply dc voltage The function returns the nearest integer of the input number (e.g., round (3.4) = 3, round (3.6) = 4) .This nearest integer multiplied by 'V' corresponds to the closed level to the reference that is generated by the inverter. Based upon the integer value one switching state is chosen at a time to provide corresponding desired voltage level at output. The reference waveform with the existing output voltage with level count 'L' as depicted in Figure 4.2. Its Implementation is illustrated in Figure 4.3.

$$Vref = m * \{(L-1)/2\} * V * sin(wt) = Vmsin(wt)$$

Where, m is modulation index

Vref is the reference voltage

Vc is the voltage across capacitor

Vm is the peak value of reference voltage

Simulation & Result

The simulation of 1 phase 9-level HCM MLI was done using MATLAB and SIMULINK. The output voltage waveform output voltage waveforms with reference waveform are shown in the figure **5** and figure 6 respectively.

CONCLUSION

In this thesis an efficient and simple PV powered water pumping system was proposed. Hybrid cascaded modular MLI was used as a PV inverter which has less number of switches than the conventional MLIs for a given voltage

level. The PV array, MPPT algorithm block, DC-DC boost converter, 9 level HCM MLI and a single phase induction motor based centrifugal water pump were simulated using MATLAB Simulink environment

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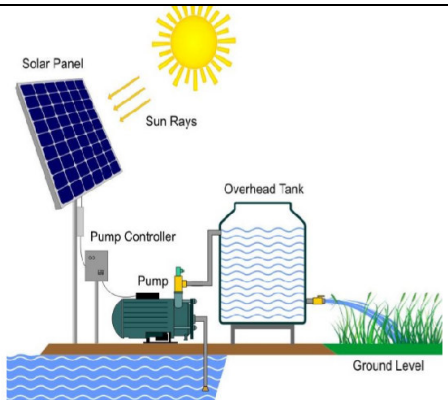


Figure 1 Configuration of a solar PV powered pumping system

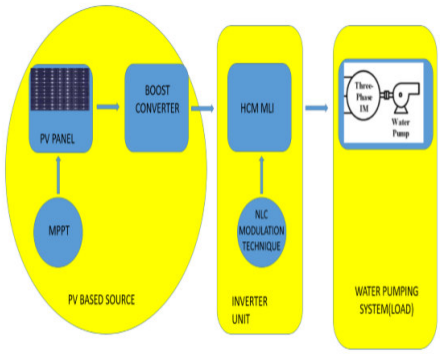


Figure 2 Proposed System for PV water pumping

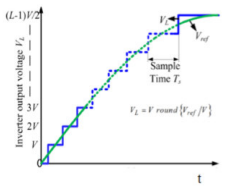
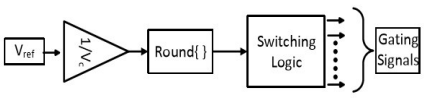


Figure 4 Waveform synthesis of level counts 'L'



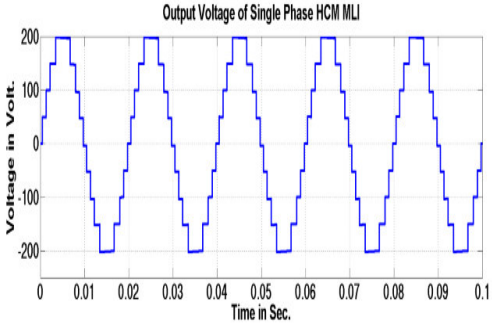


Figure 4 Waveform of Output voltage

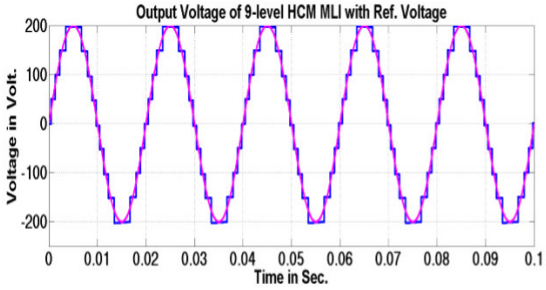


Figure 5 Waveform of output Voltage with Reference Waveform

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RESEARCH ARTICLE

Live Video Processing using Computer Vision System Toolbox

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ABSTRACT

Computer vision involves different image processing technique to process the image captured through any acquisition devices. The processing of image performed to extract feature from the image to acquire more information about the image as well as for other image processing application. For those operation MATLAB provide script functionality to perform the operation. But to avoid coding the computer vision tool box can be utilized to perform those operations. In this paper image de-noising and edge detection has been performed with the help of computer vision block set instead of long coding as script file. Both the operation are working fine and have been implemented for live execution with the help of system inbuilt camera.

Keyword: Computer vision, live video processing, image de-noising, simulink

INTRODUCTION

Computer vision is a field of computer technology which deals with understands the visual world through digital images captured using digital camera. It involve different image processing technique like enhancement, reconstruction, compression, segmentation, recognition etc for different types of application [1].

MATLAB is a numerical computing environment for development of algorithm and simulations [2]. MATLAB provide an environment which completely based on matrix manipulations. It also provides option for data visualization and other complex tool boxes for high level computation. The MATLAB allowed user to developed different image processing application using the script file. This involves the use of static images to operate and perform execution.

Simulink is a MATLAB-based graphical programming environment for system modeling and analyzing of the modeled system [3]. It provides an interface for pick and place based graphical programming with the help of block libraries. Simulink has different block set library. The computer vision system toolbox (shown in figure 1) is one of the libraries of tool boxes which used for computer vision operation [4]. This tool box can be used for both static images by capturing one frame as well as can be used with live video streaming. The video streaming is nothing but the sequence of mage frame, all the image processing operation are applied to each and every frame one by another with the help of these blocks. So that these block se allowed the user to use these block set or live image processing.

Experimental Simulation

For experimental simulation MATLAB R2014b has been used with a required specification computer system. The simulink model has been design by picking different required block for the de-noising and edge detection operation. The entire block set connected properly (shown in figure2) before execution. The 'From Video Device' block basically used to acquire image and video frames from image acquisition devices like digital camera. This block is responsible for acquiring the image or video data to simulink environment. This block is available inside the Image acquisition toolbox. It set to use the default camera of the computer system. The live streaming was captured with the help of this block. It captures the real time video with different resolution. In the current experiment it was set to 640x480 resolutions. The Color Space Conversion block converts one color space to other color space as per the specified conversion parameter [5]. Here RGB to gray scale has been chosen. The gray scale image can be obtained from the R'G'B' to Intensity block. Then both the RGB and gray scale image has been shown using the video viewer (Figure 3-4). The Image Data Type Conversion block used to change the data type of the input image to other format as specified by user. The gray scale image is converted to single data type using that block.

MATLAB Function block is used to write a MATLAB function for use in a Simulink model. The MATLAB functions which are created can be executed for simulation and generates code for a Simulink Coder. The MATLAB Function block used to insert the pepper noise to the gray scale image. In a separate m file the corresponding program has been written for the MATLAB function block. When the block gets executed by default the corresponding code will also execute. The noisy image has been shown using a video viewer (figure 5).

The median filter generally based on masking operation. It selects an m x n sub image or neighborhood and performs the median operation of the elements inside the neighborhood. The resultant median value replaces the center element of the neighborhood. This process continues till it select every sub image of that size inside the image [6]. Finally the result displayed represents the median filtered image. The median filtering is best suitable for salt and pepper type noise. This median filter block has been used to remove the pepper noise from the noisy image. The denoised live video image can be seen through the video viewer (figure6).Edge detection is the process of detecting the edge points in an image [7, 8]. This operation basically performed with the help of gradient operators and it determines the gradient magnitude value of image. The mostly used kernel is the Sobel kernel for edge detection. The Edge Detection block used for edge detection operation on gray scale frame. For another approach to display live edge detection, the edge detection block available inside Feature Detection, Extraction and Matching section of the computer vision tool box has been used for real time edge detection of the video frame. The live edge detection can be shown using the video viewer (Figure 7).

CONCLUSION

MATALB and simulink support the computer vision operation which able to perform different image processing application. In this paper the live de-noising video frame has been shown with the help of laptop camera as well as live edge detection has been shown. The de-noising of noisy image working fine with the help of median filtering block set. The SNR improved a lot after the de-noising operation. The edge detection operation also working very efficiently with the help of edge detection block set. Both the method demonstrated using the computer vision simulink block set, and it working very accurate. The most important feature is the real time live performance of the system. In the future more complex system like feature extraction of any capture video can be designed.

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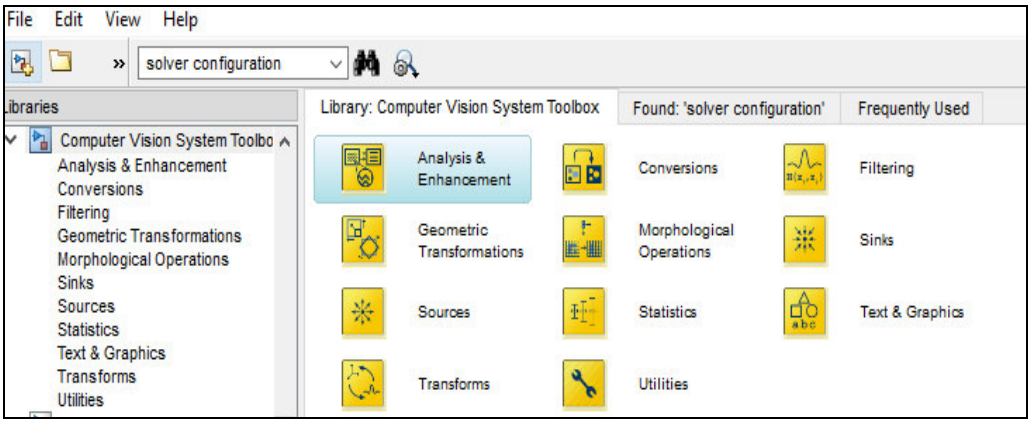

Figure 1: The Computer Vision System Tool box

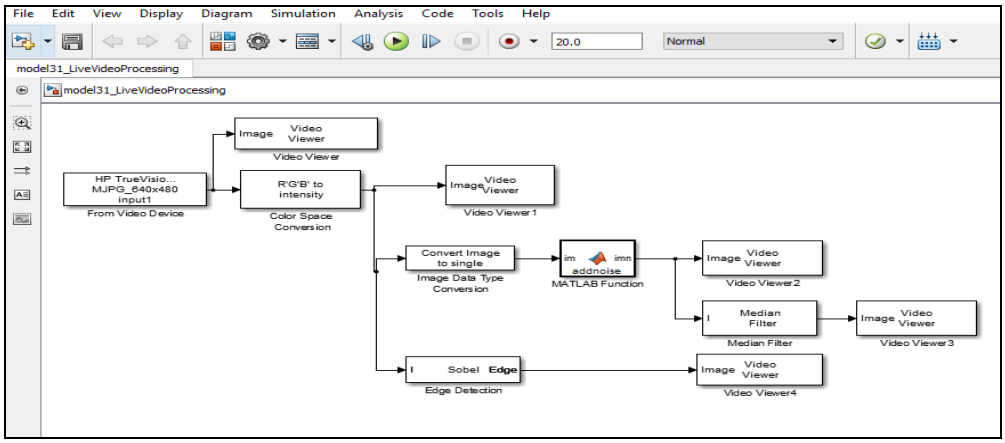

Figure 2: Simulink model for live image de-noising and edge detection

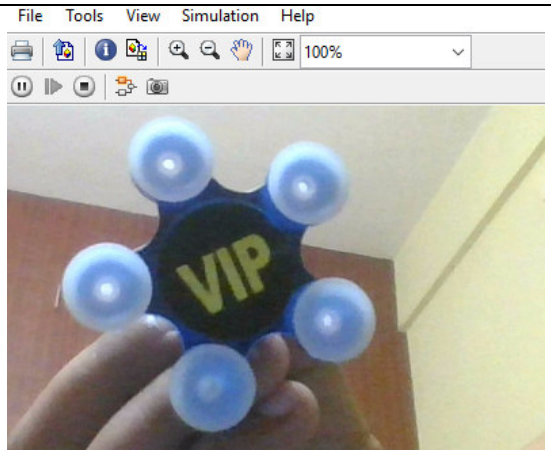

Figure 3: The RGB captured frame of video sequence

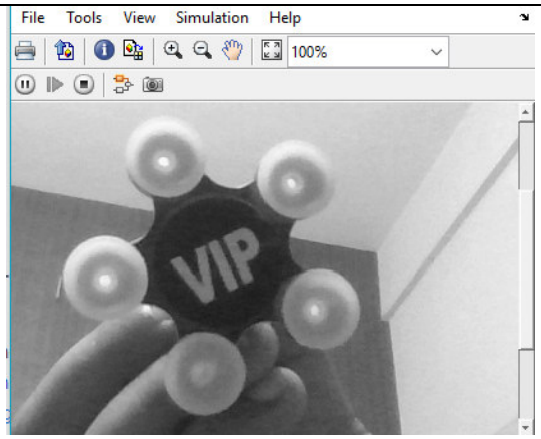

Figure 4: The gray scale image frame

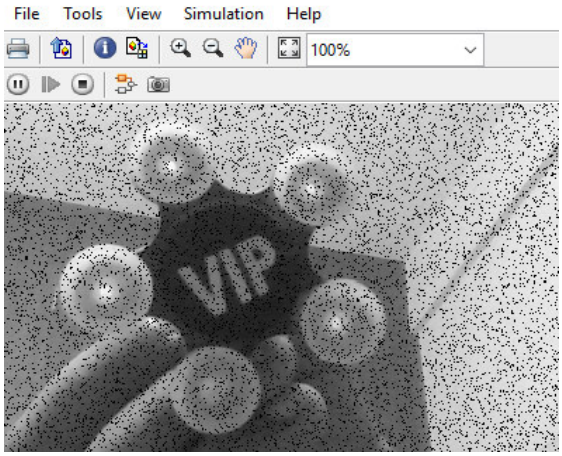

Figure 5: The image frame with added peeper noise

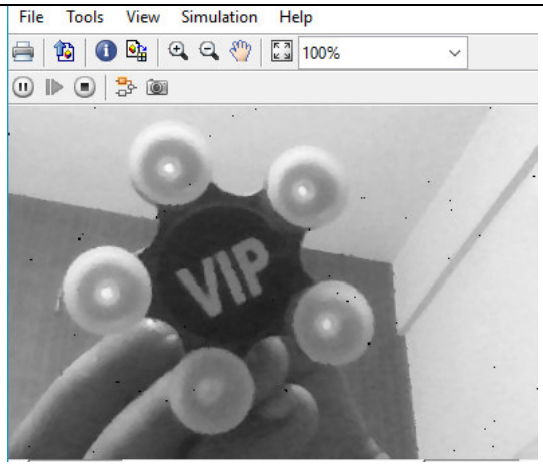

Figure 6: The de-noised image frame

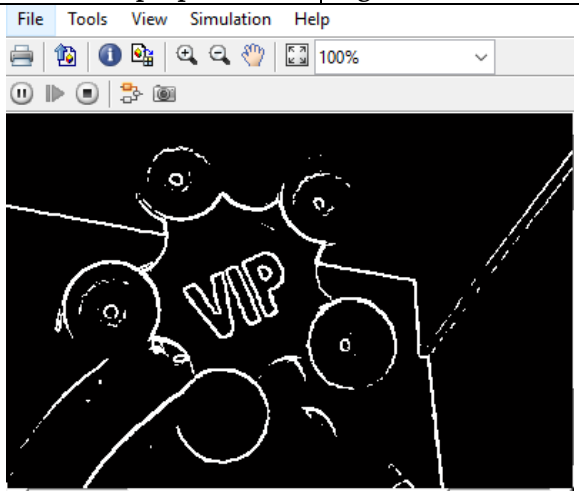

Figure 7: The live edge detection image frame

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RESEARCH ARTICLE

Modelling of Components Using Dymola for Power Grid

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ABSTRACT

Dymola's multidomain capabilities allow users to catch all applicable physics in the context of electrical engineering. Modelica's versatility enables fast nvention, design and testing of systems from rotor mechanics to power grid. It is also possible to model the entire power plant from the source of electricity, whether it is oil, coal, hydropower or other renewable sources, such as wind, All the way to the end user, via the generator and power grid. The components in the Electric Power Library provide the thermal and mechanical domains with uniform nterfaces and can be easily combined with components from other libraries to reflect electric power and actuation. Applications nclude: power grid n nominal and fault conditions, power generation scenarios including grid-connected wind turbines, multi-connected turbine generators and multi-phase generators, as well as a variety of system use examples for different use scenarios. Also deal for control design, the Electric Power Library supports multiple reference frame representations ncluding the standard nertial "abc" reference frame, as well as the Park transformed "dq0" and "dq" representations. The transformations allow efficient modeling of multiphase AC systems for both transient and stable dynamics of the state.

Keywords : Dymola, Modelica, Power system Library, PSS, Exciter,

INTRODUCTION

Modelica is an article arranged, definitive, multi-area language for demonstrating complex frameworks, for example, physical frameworks containing mechanical, electrical, water-powered, warm, electrical, or process-situated sub-segments [1]. Modelica language s intended to help viable library improvement and trade of models. This s a cutting edge language dependent on causal displaying of scientific conditions and article situated structures for the reuse of information demonstrating [1]. The Modelica language is being created by the Modelica Affiliation which s not an organization. The Modelica Affiliation has likewise built up a free Modelica Standard Library which includes around

1360 nonexclusive model parts and 1280 capacities n distinctive areas now updating the library to rendition 3.2.1. As depicted n Table 2.1 various business and free programming assets dependent on Modelica are presently accessible for industrial and scholastic use. The important differences between various applications s the interface and the solvers. While a few open-source frameworks (for example Scicos) utilize a Modelica sub-set to show segments.

In this paper, Dymola was chosen as the setting for demonstrating and reenactment. Contrasted with other Modelica conditions, Dymola s easier to use and has solver proficiency that permits enormous frameworks to be reenacted quicker. it causes clients to make a graphical portrayal of physical structures that are helpful n power framework systems implementation. Likewise, models in Dymola can be traded to the FMU design which another programming (for example Simulink) can see, which means co-recreation and trade of information with other reproduction instruments can be figured it out.Table 2.1.

Application example

This section presents an example of the main constructs used by Modelica to specify the DAEs found n models of power systems. Figures 1 and Figure 2 show a transformer model 's view of the con, text and diagram respectively. The model's graphical appearance may be designed n con view. In text view, code will describe the parameters, variables, and equations. In the diagram view, the user may drag and drop existing models (in this case, the connector model) to create a new model. When the contents of each view are changed, two more will be changed at the same time. In model creation, there are three essential concepts to be considered: the definition of class and connectors, statements and equations, and model nitializations.

Classes and connectors

Modelica is object arranged using the idea of "class" to speak to models. One class can ordinarily be viewed as a ndependent model. A "library" can be shaped by gathering essential models, and the models n library can be associated or collected to mplement new models. Associating models s by means of connectors. Connectors are unique Modelica classes, which characterize the standards for the association of at least two segments [2]. As indicated n Figure 1, connector models are utilized for the association of transformer and other force framework parts. Two models of connectors are normally utilized: PwPin connectors for electrical segments and mpin connectors for non-electrical segments.

To interface segments "electrically" by means of PwPin connectors, vr, vi and r factors are determined to introduce the genuine and maginary parts of the voltage and flow separately. To connect the factors, two sorts of connection rules are applied: the correspondence rule applies to voltage factors, and the aggregate to-zero principle applies to current factors, as demonstrated n Figure.3 and conditions.

Declarations and equations

As demonstrated in Figure 1, a Modelica model comprises of a segment on the condition and an area on contention. Model conditions are characterized in condition area. Parameters and factors are pronounced in the Assertion segment as indicated by their information type. No extra factor is characterized for this situation, so the factors in the connector model (p.vr, p.vi, p.ir, p, I) are the transformer model variable. The entirety of the announced factors is autonomous variable time work. The time variable is a worked in include that all models can utilize. Moreover, a model's conditions comply with the idea of a coordinated information stream: all factors safeguard their present qualities until they are explicitly changed, and the relation characterized by the condition must be satisfied in any purpose of time [2, 3].

Initialization of models

Prior to beginning the reproduction for a model, initialization s performed to dole out reliable qualities for all factors gave n the model [2]. The subordinates (der(x)) are respected, during this procedure, as obscure mathematical factors [4]. On the off chance that a model has subordinate capacities, at that point, the quantity of logarithmic factors is more noteworthy than the quantity of initialization issue conditions. Along these lines, extra limitations in the initialization procedure must be given. The model is initialized from a consistent state n most circumstances, which means setting dx/dt=0 as the initial condition. You would then be able to get the initial esteem x0 by fathoming f(x, t) = 0. The statement can be accomplished by inserting the initial condition n the condition area, and by utilizing the articulation start = esteem n the segment of the assertion.

Modelling of Power System Components n Modelica

This part portrays Modelica's nitty-gritty displaying methods and testing results for power framework segments. The demonstrating objective s to fabricate exact and reusable models that can fit well with different models of intensity frameworks. Since certain straightforward models (for example transports, transmission lines, transformers, and so on.) are accessible from past works [5], this investigation centers around displaying control parts n the force framework. Demonstrating is dependent on another programming which is utilized as models n request to show the segments accurately. In this examination the referenced program s PSAT, PSS/E, and Simulink. Since the working techniques for reference programming are fundamentally unique in relation to Modelica, it is important to follow another displaying approach. The measures towards positive displaying are as per the following:

1. Read the prototype specification, grasps the model's conceptual context.
2. Dentify the equations which describe the model's dynamic behaviour.
3. Write Modelica design.
4. Model nitializes.
5. Carry out Modelica model software-to-software testing against the reference model.

A few models are provided n this chapter to llustrate the baseline processes. Templates nclude:

- Synchronous generator models (Software reference: PSAT)
- Turbine governor TG1 (Software Reference: PSAT)
- EXAC1 (Ref: Software: PSS/E) excitation device
- Stabilizer of the power systems (Ref: software: PSS/ E)
- Changers to the load tap (Simulink comparison software)

Power system components modeling principles

The following principles must be followed:

- Defining the model in the most direct and easiest manner possible. Modelica allows a model to be described using other models, enabling the user to easily link models together to create a new model without converting the whole model nto equations. The first step in modeling s therefore to find the most appropriate way of expressing the model.
- Describes and explicitly states parameters, constants and variables. Constants in Modelica don't change over time and can not be modified; whereas parameters are constant over time but can be modified; and variables are varied over time and are commonly used n equations. Model style nputs and outputs have to be specified and described separately.
- Position the parameters on top of a model block sheet. To easily reuse the models, the parameters of the model must be written on the top layer of the block for easy adjustment. To be clearly described and specified.

- Parameters of the constituent components must be propagated onto the top layer, in particular for models made up of other components.
- Use the connectors as nterfaces for nput and output. Before modeling, the model nputs and outputs must be verified, and corresponding types of connectors are used as interfaces to other models.
- Choose the proper method of nitialization. One can initialize models through either auxiliary parameters, or initial equations.
- Descriptive nature of the model's appearance. The model is supposed to be one single block. Unless the model is created by connecting other models, then they have to be aggregated nto one block or symbol.
- Versions are packaged n packages. Kit s an simple way to structuredly arrange templates. Models may be grouped of similar form n one box, which makes it easier to locate a specific model n the applications.

Implementation of models n Modelica

A. Synchronous generators

This section explains Synchronous Generator modeling. in PSAT, two separate generator models are mplemented based on the mathematical models [6][7]. Different simplifications can be mplemented in PSAT generator models, and the models diverge from the basic model with only classical swing equation to an eight-order model with field saturation. Additionally the dynamics of transient and subtransient voltage are considered n the two models described n this section. In differential equations the models differ mainly forth Order.

The fourth-order generator model variables and parameters are detailed in models. Other than parameters and variables, the auxiliary parameters for initializing the variables are defined. After power flow computations the models are initialized. Upon determination of the power flow solution, v0, 0, p0, q0, and v0f are used at the generator bus to nitialize the variables. The nitial values of variables. In this model, in addition to the classical electro-mechanical model, lead-lag functions are used for modeling the inductances d and q-aixs. The dynamics of electromagnetic fluxes was gnored, resulting n a fourth order structure n the status variables π, β, e 0q and e0d. The differential equations consist of:

$$\dot{\delta} = \Omega_b(\omega - 1)$$

$$\dot{\omega} = (P_m - P - D(\omega - 1))/M$$

$$\dot{e'_q} = (-e'_q - (x_d - x'_d)i_d + v^*_f)/T'_{d0}$$

$$\dot{e'_d} = (-e'_d + (x_q - x'_q)i_q)/T'_{q0}$$

Where

$$\Omega_b = 2\pi f_n$$

$$v^*_f = v_f + K_\omega(\omega - 1) - K_p(P - P_0)$$

The voltage and current connections are defined n the equation:

$$e'_q = v_q + r_a i_q + x'_d i_d$$

$$e'_d = v_d + r_a i_d - x'_q i_q$$

Similar to the model of the fourth order, ancillary parameters are specified to nitialize the variables. The model is initialized using v0, 0, p0 and q0 flow solutions. The nitial values of each variable are described n system modelling.

Assuming a field circuit and an additional circuit along the d-axis, and two additional circuits along the q-axis, the sixth order model is obtained [This model s the PSS2B-Dual-Input PSS type of EEE which uses the power and speed or frequency combinations commonly to extract the stabilizing signal [8]. The dynamics of electromagnetic fluxes are neglected, resulting in a sixth order system n the variables of the status π, α, e0q, e0d, e00q, and e00d. The differential equations consist of:

$$\dot{\delta} = \Omega_b(\omega - 1)$$

$$\dot{\omega} = (P_m - P - D(\omega - 1))/M$$

$$\dot{e_q'} = (-e_q' - (x_d - x_d' - \frac{T_{d0}''}{T_{d0}'}\frac{x_d''}{x_d'}(x_d - x_d'))i_d + (1 - \frac{T_{AA}}{T_{d0}'})v_f^*)/T_{d0}'$$

$$\dot{e_d'} = (-e_d' + (x_q - x_q' - \frac{T_{q0}''}{T_{q0}'}\frac{x_q''}{x_q'}(x_q - x_q'))i_q)/T_{q0}'$$

$$\dot{e_q''} = (-e_q'' + e_q' - (x_d' - x_d'' + \frac{T_{d0}''}{T_{d0}'}\frac{x_d''}{x_d'}(x_d - x_d'))i_d + \frac{T_{AA}}{T_{d0}'}v_f^*)/T_{d0}''$$

$$\dot{e_d''} = (-e_d'' + e_d' + (x_q' - x_q'' - \frac{T_{q0}''}{T_{q0}'}\frac{x_q''}{x_q'}(x_q - x_q'))i_q)/T_{q0}''$$

where

$$\Omega_b = 2\pi f_n$$

$$v_f^* = v_f + K_\omega(\omega - 1) - K_p(P - P_0)$$

$$e_q'' = v_q + r_a i_q + x_d'' i_d$$

$$e_d'' = v_d + r_a i_d - x_q'' i_q$$

Turbine Governor

Turbine governors describe the primary regulation of synchronous system frequencies. Figure 5 displays the turbine governor model (TG1), mplemented n Modelica. The reference model is developed originally in PSAT. The model has three nput signals as shown n the block diagram: the actual speed of the rotor, the reference speed of the rotor, and the reference active power pref. The model output s the mechanical power Pm that s to be added to the generator. The governor controls the generator speed by comparing their output to a predefined reference. The governor regulates the speed proportionally to ts power rate when R 6=0 and R< ∞ locally. Two lead-lag filters are used n the mechanical component to stand for servo engine and reheat mechanism.

The Turbine Governor model variables and parameters are described in the system. Also, auxiliary parameters are specified to nitialize model variables. The values at the equilibrium point (e.g. 0 and p0) are the initial values of each variable. The parameter for nitialization is also explained.

The following equations could define the model:

$$p_{in}^* = p_{ref} + \frac{1}{R}(\omega_{ref} - \omega)$$

$$p_{in} = \begin{cases} p_{in}^* & \text{if } p^{min} \leqslant p_{in}^* \leqslant p^{max} \\ p^{max} & \text{if } p_{in}^* > p^{max} \\ p^{min} & \text{if } p_{in}^* < p^{min} \end{cases}$$

$$\dot{x_{g1}} = (pin - x_{g1})/T_s$$

$$\dot{x_{g2}} = ((1 - \frac{T_3}{T_c})x_{g1} - x_{g2})/T_c$$

$$\dot{x_{g3}} = ((1 - \frac{T_4}{T_5})(x_{g2} + \frac{T_3}{T_c}x_{g1}) - x_{g3})/T_5$$

$$p_m = x_{g3} + \frac{T_4}{T_5}(x_{g2} + \frac{T_3}{T_c}x_{g1})$$

Excitation system

Exciter EXAC1 is one of the models of the excitation framework worked at Modelica. The reference model was grown initially in PSS/E [6]. This model s the AC1A model of the EEE structure which relates to an exciter of the alternator-rectifier worked by field. The exciter s made out of a primary exciter alternator with uncontrolled rectifiers. The exciter doesn't utilize self-excitation, so the intensity of the voltage controller is drawn from a source not impacted by outer drifters. The diode trademark in the exciter yield, as appeared in Figure 7 [8], imposes a lower breaking point of zero on the exciter yield voltage. The model has three input flags as indicated n the square graph: generator field current FD, generator terminal voltage EC, and force framework stabilizer (PSS) signal Versus On the off chance that no PSS is mounted on the exciter, versus can be set to zero. Part yield is the voltage field EFD to be associated with the generator. Since the model is initially spoken to by square chart, It is implemented by utilizing built-up parts n Modelica, as indicated in Figure 6.

Power system stabilizer

Another important segment n the force framework s the Force framework stabilizer (PSS). Empowered with PSS, electromechanical motions can be hosed by adding the PSS yield to the excitation gadget as an extra input signal. The reference model was grown initially n PSS/E [6]. Figure 8 shows the PSS model (PSS2B), implemented in Modelica. This model s the PSS2B-Double Information PSS kind of EEE which utilizes the force and speed of recurrence mixes ordinarily to extricate the balancing out sign [8][9].

The model has two nput signals as shown n the block diagram: speed deviation (or frequency deviation) and active power Pe. The model's output s the PSS VOT HSG signal to be connected to an exciter.

Load tap changer

A load tap changer (LTC) s a device for selecting contact points along a power transformer with a variable turns-ratio (or tap changer, .e. n). The role of LTC s to regulate load voltage automatically by switching n. The representation of the LTC transformer effect s especially mportant for the study of phenomena of slow voltage collapse [10][11]. This model can be implemented in Figure 8.

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Software environment based on Modelica

Commercial software	Free software
AMESim	JModelica.org
Dymola	OpenModelica
CyModelica	Scicos
Wolfram SystemModeler	
SimulationX	
MapleSim	

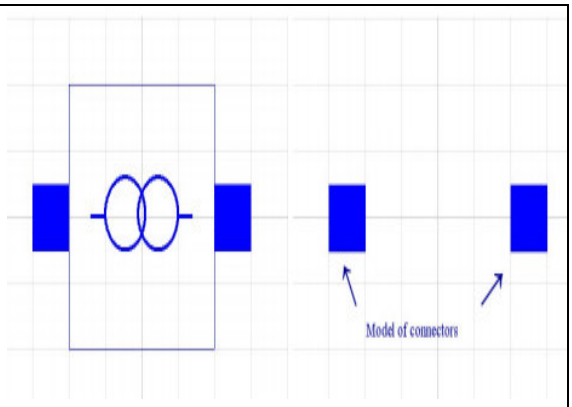

Fig.1: con and diagram view of transformer model

```
class PwTransformer2
  Connectors.PwPin p
                    a;   } Model of connectors
  Connectors.PwPin n
                    a;
  parameter Real R "Resistance";
  parameter Real X "Reactance";
  parameter Real G "Shunt conductance";
  parameter Real B "Shunt susceptance";
  parameter Real r "Transformation ratio";   } Declaration of parameters and variables

equation
  r*(G*n.vr - B*n.vi - n.ir)=p.ir;
  r*(G*n.vi + B*n.vr - n.ii)=p.ii;
  R*p.ir - X*p.ii=r*r*p.vr - r*n.vr;
  R*p.ii + X*p.ir=r*r*p.vi - r*n.vi;   } Equations
  a;
end PwTransformer2;
```

Fig..2: Text view of transformer model

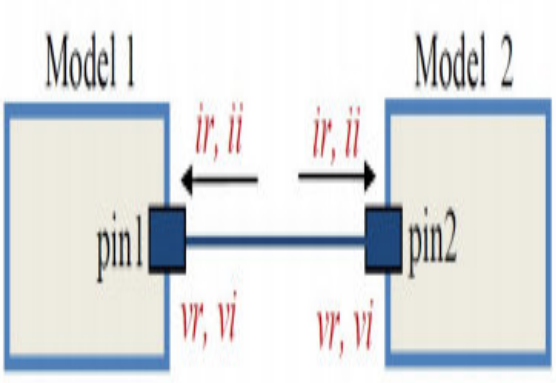

Fig.3: Connection of two models using PwPin connectors

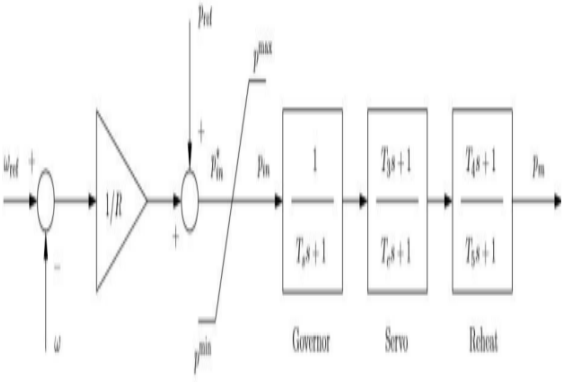

Fig..5: Block diagram of turbine governor model TG1

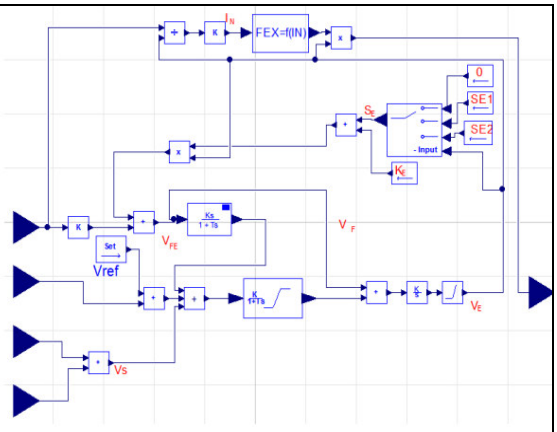

Fig.6. Excitation system model EXAC1 in Modelica

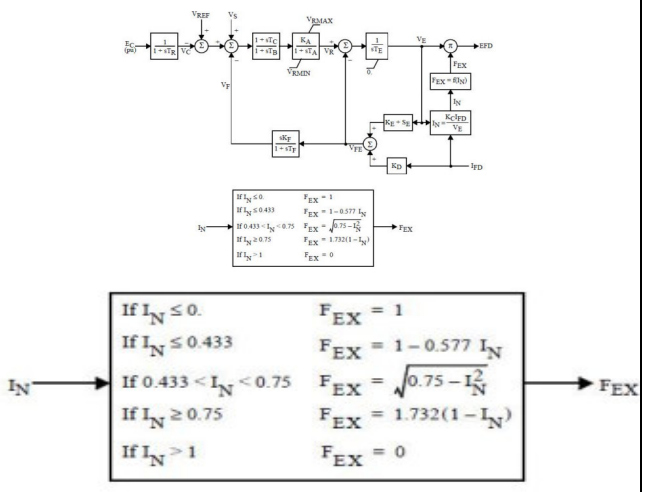

Fig.7. Block diagram of excitation system model EXAC1

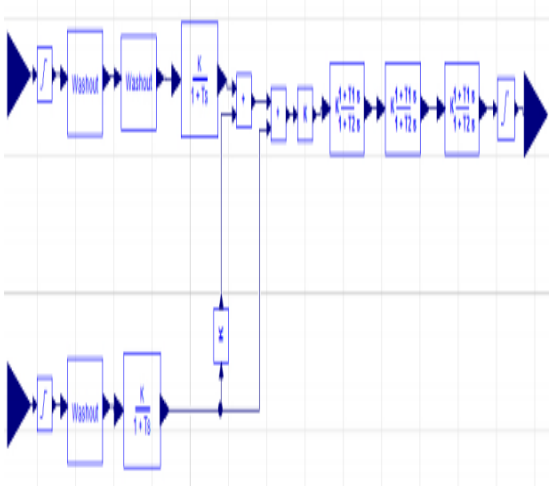

Fig.8. PSS model PSS2B n Modelica

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RESEARCH ARTICLE

Parameter Analysis of ZCS Resonant Boost Converter for High Power Application

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ABSTRACT

Recently developed zero-current-switch quasi resonant converter (ZCS-QRC) provides improved switching condition for the power transistor by reducing its current to zero prior to turn off. The turn on however, occurs, when the full input voltage is applied, to the transistor, resulting in turn on switching losses & noise. Zero voltage switches QRC over com this problem by shaping the transistor voltage for zero voltage turn on. In ZCS-QRC the transistor however suffers from excessive high voltage stress & the converter regulation characteristics & stability are adversely affected by parasitic oscillation caused by the junction capacitance of the irectifying idiode. iA inovel imulti iresonant iswitch iconcept iis iproposed ito iover icome ithe iproblem iof iQRC.The iunique iarrangement iof imulti iresonant inetwork iresults iin iabsorption iof iall iparasitic icomponent, iincluding itransistor ioutput icapacitance, idiode ijunction icapacitance i& itransformer ileakage iinductance, iin ithe iresonant icircuit. iThis iallows ithe inew iconverter ito iprovide ifavorable iswitching icondition ifor iall idevices. iExperimental iresults ishow ithat iZCS-RC iis ibetter ithen iZVS-QRC idue ito ireduced itransistor ivoltage istress, iimproved iload irange i& istability

Keywords : itransistor, izero, inetwork, iExperimental

INTRODUCTION

In ia iconventional iapplications isuch is ispeed icontrol iof ia iDC imotor, ithe iswitch iis iturned ion iand ioff ito icontrol ithe iduty icycle. The iperformance iof iDC io iDC iconversion iis ibest iat ihigh ifrequency idue ito ifollowing ireasons.

1. Continuous conduction
2. Filter size is reduced.

3. Cost is reduced.

Disadvantages of converter

1. It causes EMI problem
2. Voltage stress on the switch is increased.
3. Switching loss predominates at higher frequencies and affect the
4. optimum performance of he converter.

The switching methodologies discussed above are called hard switching as voltages and currents are forcibly interrupted when the switch is turned on and off. This causes switching losses during turned on and off.

In soft switching, the switch is turned on or off when either the voltage or current or both are zero.

In resonant switch converter, inductors and capacitors associated with the switch to cause the switch current or voltage to go to zero periodically.

There are two types of resonant converters
1. zero voltage switching (ZVS) converter
2. zero current switching (ZCS) converter

The resonance frequency is

$$w_1 = \frac{1}{\sqrt{L_r}} \times \frac{1}{\sqrt{C_r}}$$

And normalized impedance is
The resonant voltage

$V_r(t) = I_L Z, \text{ Sin } (w_1 t + a_1)$

Where $a_1 = \sin^{-1}$

The peak value of $V_{C1}$is

$V_1 + I_L Z_1$

Discussion on ZCS QR converter

- Regulation of QRC is achieved by varying the switching frequency keeping the OFF time fixed, i.e the duty ratio is altered by varying the ON period
- For the analysis of the output filter $L_f - C_f$ and load are assumed as a constant current
- The semiconductor switch is operated with zero voltage turn on and turns off
- The switch is required to with stand a forward voltage that is higher than V_1 by an amount $Z_1 I_L$
- This technique is limited to an essentially constant load application

Advantages

- The power losses during turn on and turn off become zero
- These converters have high power density and transfer efficiency
- Filter, inductor or transformer size is reduced
- The EMI is reduced during transition
- It can withstand short circuit conditions

Disadvantages

•They are regulated with variable frequency controller

•Switching loss predominates at high frequencies and affects the

•optimum performance of the converter.

From the output waveform it is seem that immediately after the diode current reduces to zero, voltage applied to the diode changes abruptly from zero to V_1. In practice such an abrupt change induces parasitic oscillations between the resonant inductor and diode capacitance as shown fig. Below.

•During conduction of b, the current through the switch and voltage across the diode are oscillatory.

•ZCS-QRC is extensive voltage stress at the switching transistor

RESULT ANALYSIS

In voltage switching converters as the switching instance is just at zero crossing the harmonics is significantly reduced. The total harmonic distortion of converter is also reduced.

CONCLUSION

The overall device life is increase due to better switching frequency Thus such arrangement will give better stability to control circuit.

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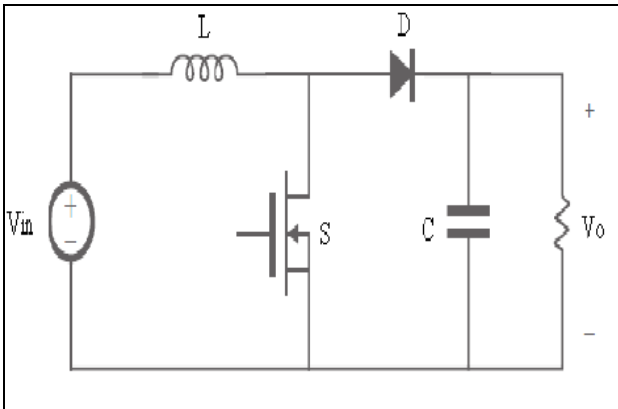

Fig: 1 Boost converter circuit

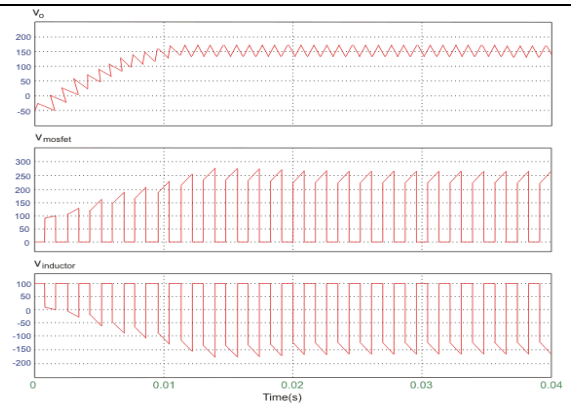

Fig: 2 Output wave form Boost converter circuit

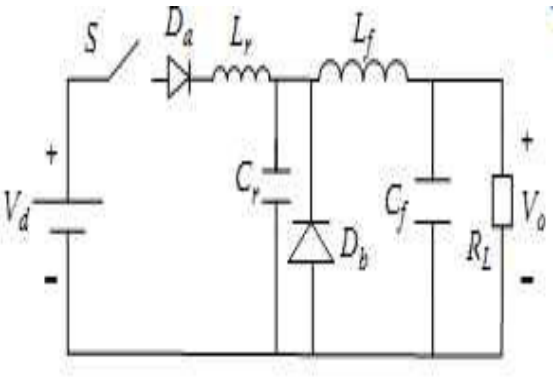

Fig: 3 NCS Resonant converter circuitC

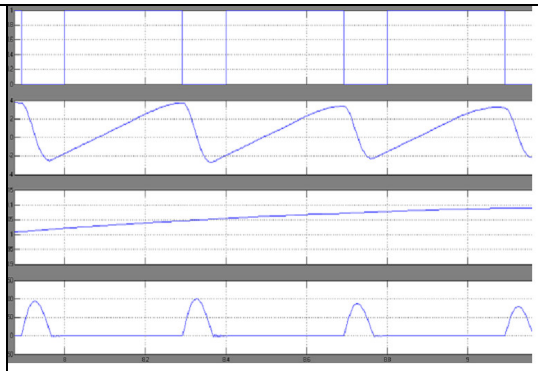

Fig: 4 Theoretical output waveform of ZCS Resonant converter circuit

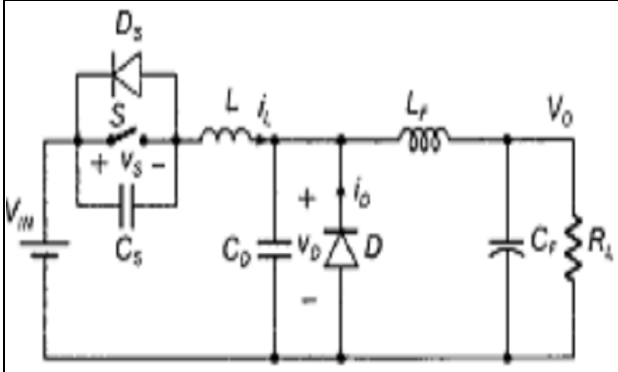

Fig: 5 circuit diagram for ZCS-RC

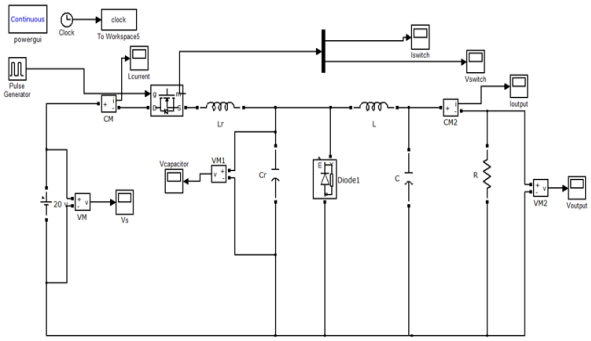

Fig: 6 Simulation Block diagram for ZCS-RC

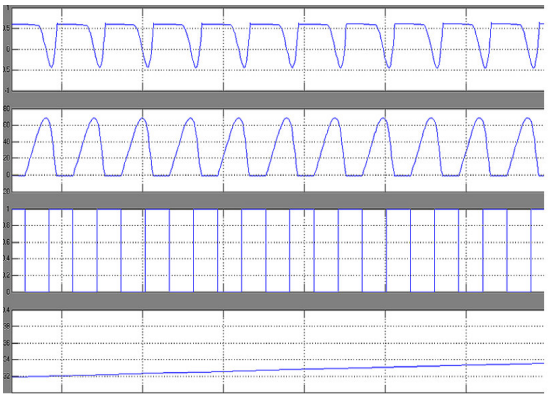

Fig: 7 Simulation output waveform output waveform of pulse, load current, switch voltage

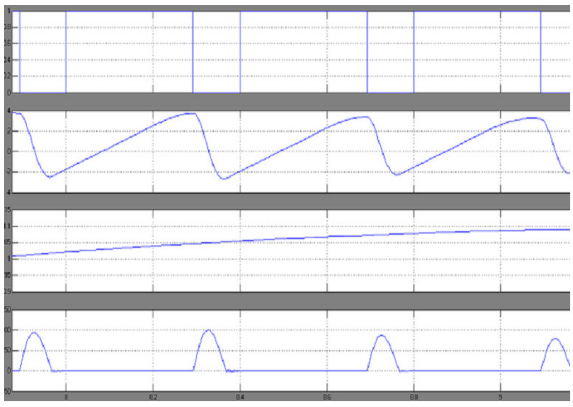

Fig: 8.1 Simulation output waveform of Switching Pulse

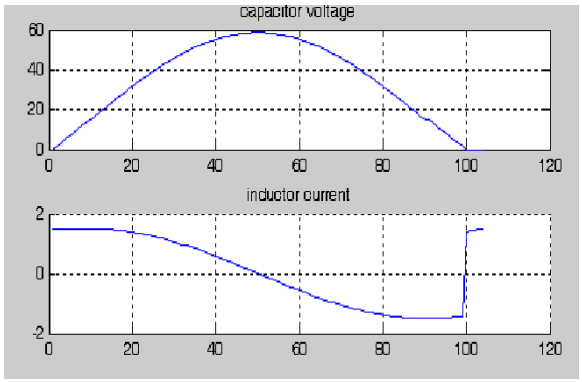

Fig: 8.2 Simulation output waveform of inductor current, capacitor voltage

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RESEARCH ARTICLE

Impact of Current Transformer Saturation in Bus-Zone Protection in High Power Transmission Network

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ABSTRACT

Zone division in Power System is critical to maintain power quality & security of system. It is also necessary for disconnecting healthy operational part from faulty part in general operating condition. The zone division in Power System is done by proper selection and placement of current transformer(CT). So when the CT becomes saturated the zone protection could not be realized due to malfunction of relay &parameter decentralization. The paper mainly focuses of CT saturation & its impact of Bus Zone protection Power System.

Keywords : CT Saturation, Knee Point Voltage, Bus-Zone Protection, Impedance measurement, Saturation Flux.

INTRODUCTION

In modern Power System protection & measurement plays an important role in stability of grid. This can only be achieved through accuracy & speed of operation. With state-of-the art development in electrical manufacturing sector the texture of instrument transformer is also modernize to fulfill the requirement, looking to recent development optical fiber CTs are replacing conventional CTs, but it has its own challenges. As the process of development is gradual, the presence of conventional CT cannot be ruled out. So for a healthy system operation fast & accurate CT operation is critical.

Current transformer is a type of instrumentation transformer which is used to convert higher level current up to a level workable for protection, measurement and control setting. It produces a secondary current which is proportional to the current in the primary.

Current transformer insulates the secondary side from the high voltage of the primary side so that the secondary side is not exposed.When saturation occurs due to fault in the transmission line, the relay that is connected to the transformer cannot operate properly.The secondary current is mainly used for the purpose of metering and protection.For protection less accuracy in CT is required as compared to the metering. In this paper distance protection system is connected with CT. So, accuracy of the current transformer not a major factor as the metering.

THEORY OF CT SATURATION

To understand CT saturation, first we have to know about the concept of working of CT, why does it saturate and what is happening after the saturation.

Working of CT

CT consists of two windings, secondary winding is around the core and the primary winding acts as a primary conductor passes through secondary. When current flows in the primary winding,alternating magnetic field is generated. This leads to the generation of alternating magnetic flux around the transformer core that passes throughthesecondarywinding.If a burden is connected in secondary, analternating voltage is created by the magnetic flux across the secondary. This generates analternating current to flow in the secondary side, which creates its own alternating magnetic field and alternating magnetic flux that oppose which created by the primary. This results in cancelation of fluxes and leaving a net flux of negligible amount in the core.

So, basically CT is a type of transformer that produces a current in its secondary which is proportional to the current in the primary.

Figure (1) shows an equivalent circuit diagram of CT. Where I_p(the primary current), I_s(the secondary load current), I_0 (the magnetizing current) N_1 and N_2 represent the turns ratio of the CT, and the ratio current $I_{st}$is the primary current divided by this ratio.

The resistance R_{ct}represents the secondary winding resistance of the CT and R_{load}represents the resistance of the load. Here R_{ct}value is constant whereas the value of R_{load}varies according to the load.

In CT the constant currentsource $I_p$drives the total secondary current $I_s$as determined bythe turns ratio. $I_s$is the current that is measured by the load ifthe CT is ideal.

Current Transformer Saturation

If an open circuited condition occurred on the secondary of CT, in thesecondaryside very high alternating voltage flows due to the alternating magnetic flux.This results in high burden on the secondary side, creates a low impedance path due to fault conditioncauses a very high primary current, which leads to the saturation of the current transformer.

When CT gets saturated they can no longer maintain the current ratio between the primary and the secondary winding. Saturation may leads to malfunction of the protection devices as the measured current does not correspond to the current on the system.

SIMULATION OF CURRENT TRANSFORMER SATURATION

Figure (2) represents the MATlab simulation of a current transformer where there is connection between the source and output voltage and current. A voltage source of 120 KV is connected to the primary side

of the current transformer through a circuit breaker. The rated current of the current transformer iss 2000/5.

The turns ratio of the transformer is repsented by,

$$N_1 I_P = N_2 I_S \qquad (1)$$

Where N_1= primary turns and N_2 = secondary turns

The primary of the current transformer is taken as 1 turn. That means seconadary current is fixed as 5A and so accornding to equation (1) , the secondary turns is 80 turns and 400 A current is flowing in the primary side.

The output current and the flux can be represented by using the scope connected in the Simulink block. By using this block we can observe the behavior of current transformer for both normal and saturation condition.

Figure (3) explains the generated secondary current of the transformer without saturation. It can be observed from the graph that the variation in curve is synchronized with time which indicates that ratio transformation is occurring in a smooth way, i.e. as per the current level in the line, the replication in reduced level as per ratio is availed for protection & measurement

Figure (4) explains the generated flux of the transformer due to the secondary current and can be measured by using the multi-meter. It can be observed from the curve that the envelope reduction is gradual with diminishing margin in positive and negative quadrant. With diminishing marginal shifting there will cause heavyfluctuation of current, this will lead to unnecessary relay actuation & circuit breaker triggering.

Figure (5) explains the influence of current saturation on the secondary current of the transformer. It clearly indicates that during saturation the peak current value reduces drastically and varies in-uniformly w.r.t. time. That is in spite of standing ratio the current value does not change accordingly as it should be.

Figure (6) explains the effect of current saturation on the flux. It indicates that the exchange of flux becomes constant after excitation flux reaches knee point voltage as shown in graph the flux increases to peak value as remains constant in positive quadrant w.r.t. time period without any variation or negligiblevariation, for which there will be no mutual exchange of flux form Ct core to secondary. Which will leads to excess accumulation of charge in CT core, resulting in heating of the core.

IV. Power system And Current Transformer with Bus Zone- protection Simulation Block

This block consists of a 120 KV line-to-line sourcevoltage, transmission line and a CT with current saturation effect on power system and distance protection system.

This paper explains the behavior distance protection system under the influence of CT saturation. The simulation of the power system contains the source and the CT. The current signal moved from the CT to the distance protection block. Its simulation graph is given in figure (9,10).

Distance Protection Block

Distance protection is designed to detect the faults which occurred in the transmission lines.The main functions included in the digital relay model are detection of faults, measurement of impedance and Zone protection.

Detection of faults

The relay allows the direct detection of the faulty phase and tripping of the appropriate distance measuring zone. Without phase selection under reach or over reach problem might occur.

Impedance Measurement Block

The impedance measurement block consists of subsystem used to calculate the fault impedance of single phase fault. The block uses an algorithm for the fault detection shown in equation (2).

$$Z_{slg} = \frac{VA}{IA+3K_0I_0} \quad (2)$$

$$K_0 = \frac{Z_0-Z_1}{RZ_1} \quad (3)$$

$$I_0 = \frac{V_s}{Z_0+2Z_1} \quad (4)$$

Where,

Z_{slg}= single line to ground Fault impedance
A = phase where fault occurs
VA= phase voltage
IA = phase current
Io = zero- sequence current
Zo = zero-sequence impedance (75 ohm)
Z1 = positive-sequence impedance (50 ohm)
K = residual compensation factor (taken as 0.9)
Vs = phase voltage during the phase to ground fault

Zone protection

The distance protection system divides the transmission line in to different zones. Zone1 covers up to 80 percent of the first section of transmission line. The setting of the next zones depends on the length of the remaining sections of the line. Zone 2 covers up to 120 percent (Zone1+20%)and Zone3 covers up to 240 percent(zone1+zone2+20%) of the first section of the transmission line.

RESULT AND DISCUSSION

Fig.9 and Fig 10 show the parameters of the designed distance protection which cover different parts of transmission line under study. The figure (9) explains the behavior of different parameters in a power system where distance protection is connected and the CT is operated without saturation. The figure 10 shows the behavior of the parameters when the CT connected to the power system in under the influence of saturation. Current saturation leads to an error in the calculated fault impedance (Zslg) and also there is an error occurred in the algorithm which is used to calculate the fault impedance. Due to this error, the distance protection is not working as it should.

CONCLUSIONS

The CT saturation could force the distance protection, because of the algorithm which is used for the calculation of fault impedance in the protection system. This algorithm is using both the current and voltage signals. The saturation effect in CT has resulted in a failure in the calculation. This error leads to the problems in functions of the protection. So the CT saturation boost the measured impedance in the system.

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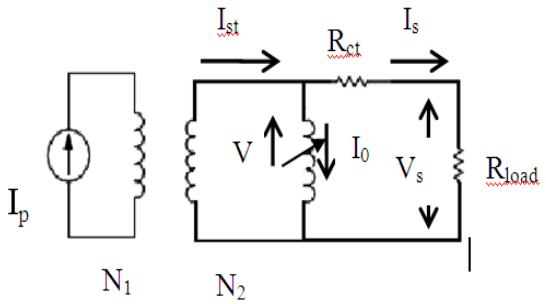

Fig.1.Equivalent Circuit diagram for Current Transformer

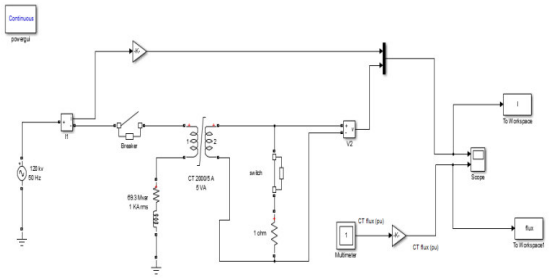

Fig. 2. Current Transformer Simulation Block

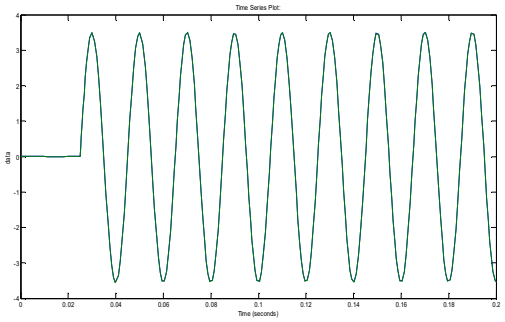

Fig. 3. Secondary current of transformer without CT Saturation

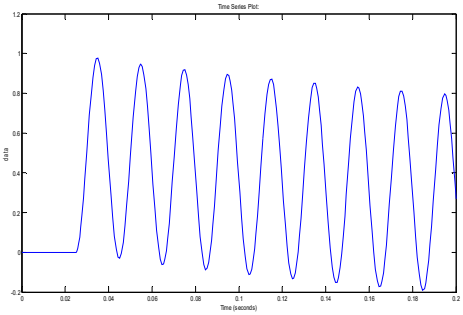

Fig.4. Current Transformer Flux without CT Saturation

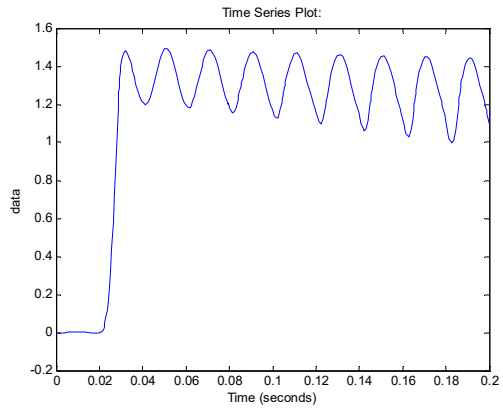

Fig. 5. Secondary current of transformer with CT Saturation

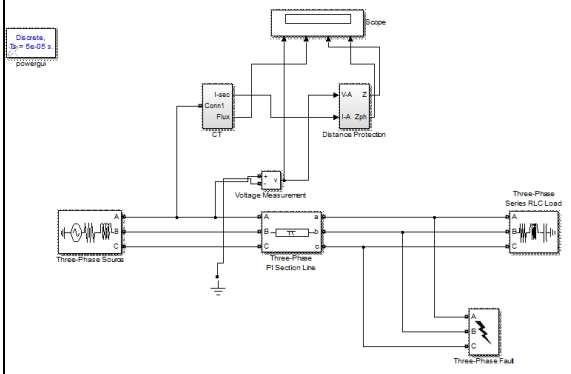

Fig.6. Current Transformer Flux with CT Saturation

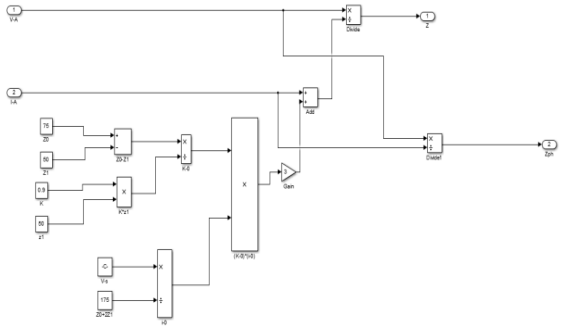

Fig.7. Power system simulation

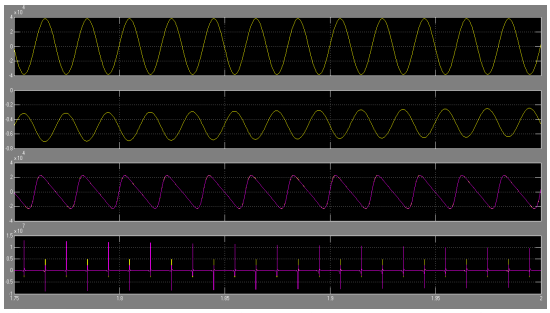

Figure 8.Apparent impedance model for SLG Fault

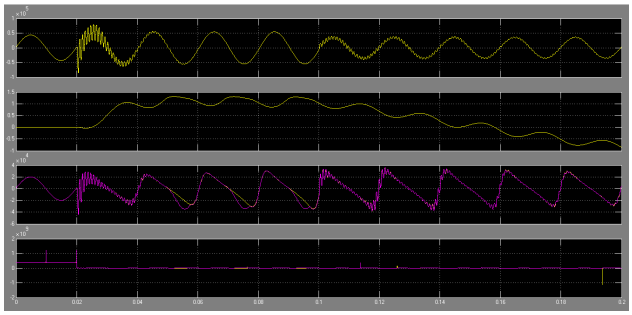

Fig. 9. Parameters with distance protection without CT saturation

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RESEARCH ARTICLE

Smart Grid Technologies and Applications

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ABSTRACT

Generally we are going to think about modernizing today's grid, we have to first of all have a clear idea about the requirement of power system in future. Smart grid is going to be the basic activity for the future developed society. Utilities across the globe are trying to find out new possibilities to bring there distribution network into the current era of digital network. By doing this they can convert the convention "power grid" into a "smart grid". By digitalization of grids the carbon foot prints of the grids can be minimized and the control over these smart grids can be achieved by new information and communication technology (ICT). When smart grid comes to picture it provides some advantages like easy integration and reliable services to the customers. A smart grid system is a system which is self-healing, self-monitoring and self-conditioning by the help of automation at each level and also it will provide reliable, security, qualitative and safe power to all consumers. This paper is a fundamental assessment of the smart grid definitions, features and technologies of the system. Moreover, this paper compressed the smart grid technologies and their advantages in various regards.

Keywords : Smart Grid, Advanced metering system, monitoring and control system

INTRODUCTION

The basic idea of smart grid is to achieve reliable, control over the flow of power or good power management. The information can be processed to re-route the electricity around the problem spot until the problem is solved. The smart grid can accommodate solar and wind power into the conventional power system. Dynamic tariff can be employed by the use of smart grid technologies. The smart grid is a automated system in which the system is capable of rapidly respond to the changes in condition. The smart grids are predictive and forcastive in terms of predicting the equipment maintenance time and forecasting the life of equipment. Today's power system is designed

for one way transmission of power from the generating stations to the consumers. But in the future it will be two way systems where small distribution units are distributed over the whole country and smart grid is the best solution to serve the problem.

SMART GRID EQUIPMENTS

Modernize smart grid can be achieved by, a wide range of technology which is to be developed and also it should be implemented. The technology are generally grouped into following areas:

Intelligent devices: Intelligent devices should be able to understand and decide at when and which moment to consume energy based on consumer load demand. In this way, these devices lead to go away from decreasing in peak loads which have an impact on generation of electrical costs. For example smart sensors(moisture, temperature sensors, etc).

Smart meters: Smart meters avails two-way communication between power distributers and load end consumers for automatic data collection of billing, detection of equipment failure. It also provides security and load control function.

Smart substation: Substation are used to control and monitor the critical as well as non-critical operational data such as status of power, performance on power factor, breaker, security, safety, etc. Substation are used for transferring voltage from one place to another that provide reliable and safe transfer of energy.

Integration of communication: It is the best part of smart grid technology i.e. integrated communication. It is faster as compared to real time operation of system. According to fulfil the need of consumer demand, communication can be like PLC, SCADA, BPL.

PMU (Phasor Measurement Unit):- It is used for the measurement of electrical waves on electric grid by using a common time source for synchronization. The time synchronizer allows real time measurements of multiple remote measurement points on the grid.

FEATURES OF SMART GRID TECHNOLOGY

- Advanced metering infrastructure system
- Consumer side coordination
- Improvement in transmission line appliances
- Distributed management system
- Information and communication technology
- Combination of renewable energy
- Monitoring and control system

Advanced metering infrastructure system

AMI describes about the two-way communication control and allow consumers and public servant to get the operation of real time cost and energy consumption. It specifies energy loss and finds the location where the electrical theft has occurred[2-3].The system can improve public service operation and help the development of AMI data management to enhance customer reading. AMI provides a fundamental link fixed between the network, customers with their loads and generation as well as storage space resources through the merging of different technologies such as intelligent evaluation, starting zone system, coordinate exchange, data management application and institutionalized programming interface [4]. In the execution of AMI the risk of communication, which is a

specific aspects consolidated in the smart grid and evil the national economy, general security, government conviction and public protection with environmental reliability [5]. As a result, the system security prerequisites must be proposed and distinguish which electrical network security goals are planned to be expected [6].

Consumer side coordination

Consumer-side coordination updated to monitor electrical consumption at the consumer level such as industrial and residential level. There are some points which are committed consumer's side coordination that are[7-8]:

- Energy storage device
- Energy management system
- Intelligent electronic device
- Distributed generations

The monitors that are used in home are pre-paid cards, smart electronic and electrical devices and cargo storage which could speed up the energy efficiency and consumer's demand [9]. At the side of end customers, the customers reduce their energy consumption in the cause to need the power grid. When we go to see the side of manual-to-customer reaction, the programmed, the internal controllers and the evaluated devices are associated with the energy management techniques or controlled by utility program and system supervisor[10].

Improvement in transmission line appliances

Different types technology that are used in transmission line to improve the controllability, ability to exchange and decrease in energy loss. There are some applications that have occurred are[11-12]:

- Flexible Ac transmission system(FACTS)
- High voltage DC system(HVDC)
- High temperature super conductors(HTS)

Distributed management system

DMS function is through processing of real time operation; smart meters, advanced sensors for [13]:

- Detecting fault location
- Improvement in energy management
- Optimizes voltage and reactive power
- Maintaining the voltage level
- Reduce interruption and repair time
- Reset the power supplies automatically

Information and communication technology

The work of ICT is to assist the communication of data for the activities granted and continue during interference. ICT is not to concentrate the communication network that are used in privately (metering work system) or public (mobile phone, link and web count)[14].

Combination of renewable energy

Renewable energy assets spread at various level of energy network: Extensive scale renewable power source assets at the transmission level, medium scale appropriation and little scale in the customer's parallel structure[15]. The capacity to control and dispatch remains the principal challenge for the for the reconciliation of renewable power source and energy assets distributed in the activity of electrical system. Both electrical and thermal energy storage plans can reduce the effect of variable renewable power source for wind and solar energy. Distributed generation integrated can enhance the power quality of power network and decrease the substantial loads[16-17].

Monitoring and control system

There is huge area of monitoring and controlling all parts of the power system and continuous execution through interconnection inside extensive geographic areas and enhances the role of power system and execution to help through framework administrator to understand them[18]. The progressed working frame work equipment including the broad area situational mindfulness, wide area monitoring framework and wide area versatile security, control and computerization, keep up a separation vital power outages and encourage the mix of variable sustainable power source assets. Also the information created by the monitoring, estimation and control frameworks of the expanded area could also encourage the activity of the structure together with [19]:

- Reporting on the decision making process
- Attenuation is extended area dispersion
- Improved transmission capability with reliability[20]

APPLICATION

- To improve the adeptness of transmission lines
- Cost reduction
- Reduction of peak demand
- Quick recovery after a sudden breakage/disturbances in the lines and feeders
- Smart grid possess the ability to be integrated with renewable energy resources on a large level which leads to sharing of loads and reduction of load on large scale.

BENEFITS

1. Reduction in carbon emission
2. Better quality of power
3. Better supply for consumer demand response
4. Increase in demand for energy
5. To integrate isolate technologies
6. To protect electrical network during emergency situation.

ADVANTAGES OF SMART GRID

The advantages of smart grid network can increase the operation of the system and it consists of:

Reliability: - The rate of decreasing the interruptions and the quality of energy. Also to reduce the possibilities and there is a penalty for generalized blackout.

Efficiency: To minimize the losses, cost to generate, for transportation purpose and consuming the electricity.

Security: To protect against cyber attack and natural disasters, decreasing in the chances of possibilities and consequences of assaults caused by imitate fraudulently and also by causing sudden great damage or failure in system.

Safety:- Decrease in fault occurrence and death toll from network related events in general.

Economy: Keeps prices in low electricity cost reducing the total amount paid by the consumers on the network, creates new jobs and stimulates total national production.

DISADVANTAGE OF SMART GRID

1. Availability of continuous communication network.
2. Due to sudden change in situation, smart grid network or performances become challengeable condition in this system.
3. The cost of smart meter become more expensive as compared to traditional old electricity meter.
4. There is some possibility of hacking the smart meters which can be used to increase or decrease in consumer demand.

CONCLUSION

This paper is a fundamental assessment of the smart grid definitions, features and technologies of the system. Furthermore, the contrasts between a conventional grid and an intelligent grid analyzed. Moreover, this paper compressed the smart grid technologies and their advantages in various regards. Energy management methodologies, challenges, and implementations are reviewed in this paper too. This work has tired the development of the smart grid from the need to modernize the electric grid. At last, the conventional network was limited and required more capacities. The features and characteristics of intelligent grid systems have recognized. This paper displayed the intelligent operation of the key and related technologies and distinguished the assessment activities, challenges, and issues spinning around them. There is opportunity about circumstances in the regions of time arrangement expectation in smart grids, reliability, and power quality examinations, energy flow optimization, battery frameworks, cloud assembly, and energy integrating sustainable on an extensive scale. Indeed, even the issues and challenges recognized as information security, physical and
Cybersecurity, test system barrier and the automation of the delivery system can be great beginning stages for future research.

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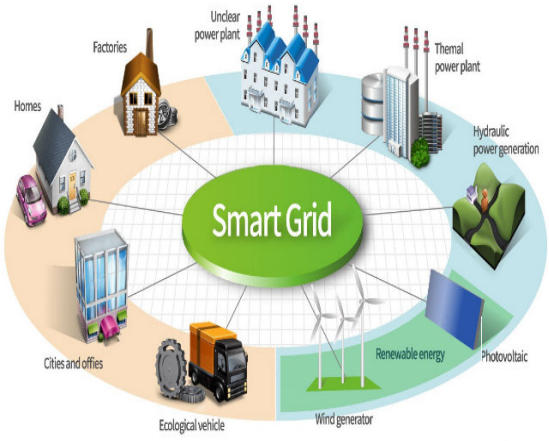

Fig.1: Phasor Measurement Unit

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RESEARCH ARTICLE

A Study on English Language Proficiency of Business Executives (Mid level) from selected Corporate Houses in India

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ABSTRACT

As industries grow and begin to globalize their products and services, employees need to be equipped with effective communication skills and English has emerged as the language of international communication. This has accentuated the need for good English language communication skills. Most employees who join business organization possess good technical knowledge and skills but there is a perceptible lack in their ability to communicate fluently and effectively. English language proficiency is integral to inter-organizational and intra-organizational communication. Employers consider communication skills to be one of the important skills for effective performance at work. In the corporate sector the language used for communication needs to be clear, direct and simple and responses need to be quick and prompt. Lack of language skills can be seen to have a negative impact on an employee's accessibility to communication networks; the possession of the relevant skills can facilitate inter-unit communication flow. The study is an attempt to identify the current language skills of the business executives and difficulties they face during the use of the four skills such as speaking, writing, reading & listening in English. Special attention will be paid to the relationship between executives; sociolinguistic backgrounds and their ability to use English in their jobs.

Key Words: Business Executives, Sociolinguistic Profiles, Corporate Sector, Language Skills, Speaking, Reading, Writing, Listening.

INTRODUCTION

Although proficiency in English is essential for business executives as mentioned above, there are many business executives in India, especially with mother-tongue or regional medium background, who have difficulties in coping with the current requirements of the English language. These business executives include professional students who

are going to step into the realm of business, self-employed professionals, 'pre-experienced' (or 'low-experience') and, sometimes, 'job-experienced' (Ellis, M. and C. Johnson: 1994:5) executives.

For Instance, there are several management, finance, marketing and engineering graduates struggling to secure a suitable job in an organization because they are not proficient in English. Similarly, there are also pre-experience business executives with English medium background who do not have the required competence in English to transact their business dealings. There are also job-experienced business executives who are not proficient enough in the use of English. Usually, job-experienced learners gain the required knowledge in the use English because of their practical experience on the job. However, there is no guarantee that pre-experience learners will be competent in the use of English once they acquire a few years of experience on the job. As Singh (1998:8) observes, it is assumed that the candidates will pick up English as they go along with their relevant job. It is true that some executives benefit from the use of English in real life communication situations, yet they cannot become confident users of English, despite an adequate interactive environment in English . Many factors inhibit the development of their use of English. These factors include their inexperience in the use of English due to the grammar-translation based schooling in English, hesitation, fear of ridicule from peer group or buyers, etc.

LITERATURE REVIEW

Training in business English in the Indian contexts has been a little researched area in India. The research done in business English does not focus on the actual language need of employees of their on-the-job work performed. As mentioned earlier not much research has been done in areas of corporate language training.

Usha Kumar (1978) analyses the letter writing skills of commerce student. Her study aims at making the reaching of an English purposeful by giving it a vocational bent and relating it closely to the demand that are made on it by the students of commerce. Kumar in her study '*English for Business'* states that '*no serious attempts have been made to assess the need for English in business'*. English is not given enough importance at the graduate level in commerce with the results that it has become an accessory.

Kumar (1978: 80, 90) also mention the different between 'education' and training. She write, "while the language syllabus in a school of a humanistic model i.e., education oriented, in colleges it should be of a technical model i.e., training oriented."

Aim of the study

Many business executives in India do not seem to possess adequate communication skills in English and, consequently, do not appear to be satisfied with the way they are dealing with people and work on their job. A business executive may have a clear business vision, business strategy and an adequate preparation for the new challenges in the ever-changing scenario of business environment. But, if he does not possess adequate communication skills in English, it is very likely that he may not be able to achieve his business goals.

There is no specialised academic course in English at undergraduate and postgraduate levels for students who wish to pursue a career as business executives in their chosen fields. The initial induction training imparted to business executives in some organizations usually does not focus on communication skills in English. Therefore, there is a need for a specialized course in English for business executives in India. And, there has been very little research in India which has focused on all four skills, viz. speaking, writing, reading and listening skills, keeping in mind the sociolinguistic backgrounds of business executives. These factors play a significant role in the business executives' ability to use English. Therefore, a specialized course for business executives with a reappraisal of the course objectives and content seems to be necessary The present need is to provide functional competence in English to business executives, in a limited amount of time with practical classroom methodology so that their lack of functional competence in English does not impede their progress on their job. Therefore, the present study sets out to:

Re-identify the English language needs of business executives in the present changing scenario

Due to the constraints of time and space, the present study is, however, restricted to the needs of the business executives working in different national and multinational companies located in Raipur, Nagpur, Hyderabad and Bangalore only where executives from different parts of the country work.. The study is also based on certain assumptions which are described in detail in the following section.

Importance of English for business executives

English is very essential for business executives for various reasons as mentioned earlier . Although various studies focused on the productive (i.e. speaking and writing) skills only , the present study emphasizes the fact that the productive skills as well as the receptive (i .e reading and listening) skills are equally important for business executives, as a majority of the executives felt it so (see table 1 below). It is felt that the rapid changes in the business environment are the main reasons for bringing about equally significant demands for reading and listening skills. Indeed, the productive and the receptive skills usually do not exist in isolation from each other, but are interrelated with each other.

Further, a business executive is expected to speak fluently, write effectively, listen and grasp attentively, read and comprehend accurately and quickly, but it was found that many executives had difficulty in using English in their job. Their specific difficulties in their job are discussed below.

Difficulties business executives encounter in English

It is evident form table 1 above that English is very important for business executive and a majority of them do use English at work. However, it was found that out of the sixty business executives interviewed, 38% (i.e. 23 executives had difficulty In speaking, 38% in writing. Similarly, many of them also had difficulties in listening and reading in English as the following table shows:

The nature of difficulties the executives face in the use of English and the reasons for the difficulties are discussed below in separate sections.

Speaking: Common difficulties

Some of the common difficulties business executives encounter while speaking in English, as the following table indicates, are speaking grammatically correct sentences, using appropriate vocabulary, speaking fluently, speaking with correct pronunciation and speaking with confidence.

A majority of business executives who had difficulty in speaking in English said that inadequate knowledge of grammar was the major reason for their difficulty. Similarly, among the 23 executives who had difficulty in speaking, 96% of them (i.e. 22 executives) found it difficult to speak in English because of inadequate vocabulary.

The underlined sentences in the conversation shows the ignorance of the business executives about correct grammar and syntax.

Q. Do you think you are not able to manage your business satisfactorily because of your lack of fluency in English?

A: Yes customers feels happy when we speak in his own language. Because, he could understand very deeply about the product when we explain in his own language only .Generally, customers influences when a shop owner or a businessman approaches, he would like to have been addressed in his own language.

Q: You said you have problem in speaking in English .Then, how do you manage your English when you have to speak to your important customers in English?

A: I'm managing with simple English. If I am not expressing my thoughts, I am always switch on native language.

Q: Could you just tell me how much and in what way English is important to you in your job?

A: Of course, it is very much essential for a professional like… English is very much important as it is an universal language which can be communicated in a better way.

Q. You've mentioned in the questionnaire that speaking in English is somewhat difficult to you, so, does it affect your job to some extent?

A. In my case it is somewhat different as I said because in my school and college days I was not so interact with students who are having good conversation in English and as I studied in a government school there was no opportunity to develop my English. If I could have been from convent or standard school where speaking in English is compulsory there might be a chance for commanding myself in the language.

Q: You've mentioned you have also some difficulty in reading. then, it affect your performance on the job while you correspond through e-mail ?

A: Not much. Because I would have been able to speak or write good English ,it would have been more impact on the receiver's end rather than at my end.

It is evident from the above examples that some executives lack adequate knowledge in grammar and vocabulary. It is also apparent from the above that the errors in grammar are part of both complex as well as basic grammar rules.

Further, their difficulty is compounded by incorrect pronunciation, poor knowledge of basic grammar, lack of confidence, etc. Among the 23 executives who mentioned that they had difficulty in English , the data suggests (see table 3) that 87% of them (i.e. 20 executives) found it difficult because of lack of fluency, 78% (i.e. executives) because of incorrect pronunciation and 57% (i.e. 13 executives) because of lack of confidence.

Writing: common difficulties

A business executive who is part of the middle or top level management in an organization is expected to possess good writing skills in English. However , the data indicates (see table 2 above) that out of the sixty business executive interviewed, 38% (i.e.23 executives) found it difficult to communicate in writing properly. Surprisingly, all these 23 executives who had difficulty in writing said that using appropriate vocabulary was their main problem. Of these 96% (i.e. 22 out of 23 executives) indicated that writing grammatically correct sentences was their main difficulty .Similarly, 74% (i.e. 17 out of 23) mentioned sequencing of sentences and 52% (i.e. 12 out of 23) mentioned organizing paragraphs and using appropriate sentences to close a letter as their difficulties in writing in English. The following table sums up these details:

The following are some examples of sentences which contain errors of vocabulary and grammar used by some of the interviewees, these sentences are taken from both their work places and the answers they wrote in the questionnaire 1

The manufacturing facilities existing at the time of visit of your survey team was lacking to cater the needs of our customers…

If you starts this proficiency course that will be helpful business executive. because they will learn…

We look forward to hear from you a positive response….

We herewith sending a proposal relating to….

We are requested to go through the letter and send your consent for above proposal.

We can attract the parties by writing this type of drafting it is necessary are for exclusive business executives.

Every parents should encourage their wards to speak in English by conversing a minutest matter in English…Simply sending their ward in a public school won't make their sons/daughters English literate.

Proper information cannot be obtained by filling up this questionnaire. This kind of method may required a little changes . Ex surveyors shall be in front of responsee and note the a clear ideas from the person whom he wants to be interviewed.

Having discussed the speaking and writing skills of the executives, let us now move on to another important area---the reading skills of the executives.

Reading: Common difficulties

From the data it is evident (see table 1) that 88% of business executives (i.e. 53 executives) considered reading skills as important to them on their job. Some of them mentioned that they often browsed the internet for information related to their business activities. Most of them also mentioned that they read technical or professional journals, magazines, books business newspapers, the usual business correspondence such as letters, fax and e-mail.

However, the data indicates that out of the sixty executives interviewed, 28% of them (i.e.17 executives) had difficulty in reading comprehension (see table 2). Their responses to certain questions in the questionnaire were neither appropriate nor relevant. That is, they were not able to grasp the content of the questions properly which reveals their inadequate reading skills. For instance, some of their responses to certain questions were as follows:

Q: When are you required to speak in English on your jobs?

Q: Which of the following functions/tasks do you (have to) person through SPEAKING in English on your jobs ? And how frequently do you (have to) perform them ?

A: In today's competitive environment speaking in English is most essential.

Similarly, in the following context, the reader instead of writing about the nature of difficulty wrote about the way he communicated in English:

Q: If you have a difficulty in speaking in English, what are your difficulties?

A: I communicate fluently with people with an intention to make them understand.

In the following two instances again, the reader has failed to understand the key words "what reasons "in the given question:

Q: what do you think could be the reason(S) for your inadequate oral communication skill in English?

A: Every time, at every level I try to improve my communication skills.

Q: what do you think could be the reasons (s) for your inadequate written communication skills in English?

A: Yes, please conduct a course.

Having discussed the difficulties related to speaking writing and reading skills of the executives, let us not discuss the difficulties related to the listening skills of the executives.

Listening: Common difficulties

Almost 92% of business executives (i.e. 55 executives) felt that the listening skills were important to them (see table 1) Business executives have to listen to and grasp quickly what their customers or clients, superiors, colleagues, etc. say to them. They listen to lectures in formal seminars and meetings as well. They also have to listen to railway announcements, flight announcements, etc. apart from listening to the radio and television.

Out of the total sixty executives interviewed, 32% (i.e. 19 executives) mentioned that they had some sort of difficulty in listening comprehension (see table 2).

The data indicated that some of the common difficulties business executives faced in listening comprehension was that they were not able to understand quickly the speaker's pronunciations, sentence structure and communicative

value of the utterance. Inadequate vocabulary was also one of the reasons for the executives' difficulties in listening comprehension.

Some of the interviewees also felt that the difficulty to listen and comprehend quickly increases as the speakers usually vary in the way they speak because of the differences in their mother tongue, educational background and geographical background,

CONCLUSION

The importance of a specialized course in English for business executives cannot be denied. And, rightly so, a majority of the interviewees, that is, about 80% (48 executives) indicated that there should be specialized course in English for business executives.

On the other hand, it is surprising that only 12% (i.e. 7 executives) had an induction programme / initial orientation training programme in their organizations which included a course in English. They also indicated that they benefited a great deal out of such a training course which aimed at all the four skills, namely listening, speaking, reading and writing.

Similarly, those who said there should be a specialized course in English for business executives also indicated that such a course should comprise all the four skills.

Some of their responses in this regard, in their own words, are as follows:

A proficiency course in English is very helpful to business executive. They can improve their listening, speaking, reading and writing skills

People should be trained in the ways to address colleagues, seniors and clients. For Example, in our country many executives use the word "sir" to every sentence while speaking to their superiors. Thus business executives also need to be trained in communication skills.

Even though most business executives come to business mainly after their graduation, it is not ruled out that some may come even without any formal education and rise to the level of top management. Therefore, I feel, there should also be separate English language programme, specially designed for business personnel without any formal education.

If there is a good course in business English it is useful to people like me. We can improve our English and deal better in business transactions. However, such a course should be very practical. It should also emphasize writing, reading and listening practice.

The above responses reveal the significance of a specialized course in English for business executives. It is also clear that such a course should comprise all the four skills, viz. speaking, writing, reading and listening.

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Table 1: Importance of English language skills for business executives

Language skills	Important	Not important
Speaking	95%	5%
Writing	97%	3%
Reading	88%	12%
Listening	92%	8%

Table 2 : Business executive's competence in English

Language skills	Not competent	Competent
Speaking	38%	62%
Writing	38%	62%
Reading	28%	72%
Listening	32%	68%

Table 3:Common difficulties business executives encounter while speaking in English

Nature of difficulty in speaking in English Response	
Lack of sufficient grammar knowledge	97%
Poor vocabulary	96%
Lack of fluency	87%
Incorrect pronunciation	78%
Lack of confidence	57%

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RESEARCH ARTICLE

Approaches to English language curriculum for English for Science and Technology (EST) students: Implications for teachers and learners

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ABSTRACT

English language plays a pivotal role in the academic and professional careers of students, especially those pursuing graduate courses in the areas of sciences and technology. Due to the emergence of globalization and commercialization, a lingua franca is the need of the hours and English language has emerged as an alternative for the trade and commerce language across the globe. Thus, there is a significant need to ensure that language curriculum for science and technology students must be based on their language needs and requirements. The paper makes an attempt to define language curriculum in the context of science and technology and highlights some implications EST teachers. In the process, three approaches to language curriculum has been discussed. Process approach has been suggested to be adopted in designing EST curriculum which would ideally encompass all the best features of the three approaches.

Key words: EST, Language Curriculum and ESP students

INTRODUCTION

The paper begins by describing what the basic features of curriculum. A broad discussion has been attempted to find out the appropriateness of the given explanations. After a thorough discussion on curriculum, a detailed discussion has been made on various approaches to language curriculum design and provides rationales for the relevance of process approach for EST students. Further, a few suggestions have been offered to the EST teachers for successful delivery of the curriculum.

The concept of a language curriculum

The word 'curriculum' has been used differently by different experts in different ways. In its narrowest term the word curriculum is synonymous with syllabus, but in a wider sense it is more than a list of subjects, rather it

includes planning, implementation and evaluation of educational programme.Kelly (1989) provides a wide-angle view of language curriculum.

> "…the intention of the planners, the procedure adopted for implementation of those intentions, the actual experiences from the people resulting from the teachers' direct attempt to carry out there or the planner intention and the 'hidden learning' that occurs as a byproduct of the organization of the curriculum, and, indeed of the school". (Kelly, 1989, p.14)

It is significant to note that curriculum in a broader sense in not a list of topics to be transacted in the classroom but there is a 'hidden learning' which highlights that the focus of a curriculum is not on 'teaching' but in the process of learning the set objectives. Nunan (1988, p. 158) also supports a broad view of curriculum.

> "…the principles and procedures for planning, implementation, evaluation, and management of an educational programme. Curriculum study embraces syllabus design (the selection and grading of content) and methodology (the selection of learning tasks, and activities".

Nunan (1988) believes that curriculum is not simply a list of subjects but it entails many more aspects i.e. planning, it may be carried our according to the needs of the learners; implementation, it takes care of appropriate way of enacting a curriculum; evaluation, it helps us how effective the earlier two principles are and finally management of the whole educational programme. It has been highlighted from the definition that curriculum goes beyond classroom happenings; it is beyond teaching and learning. Nunan (1988) not only focuses on the planning part of the curriculum, rather the process and procedure of implementing curriculum.

According to Richards (2013), 'The Forward Design Process' focuses on the linear approach to curriculum design where the content is pre-determined prior to a course delivery and it is The graded from simple to complex. It focuses on the teacher centred approach to classroom where teachers are expected to present explicit rules. However, The Central Design Process is activity-based and do not follow a linear progression. It is a process approach to language curriculum, where the content and sequence evolve in the classroom. Meaning is given more importance in this approach than accuracy and thus activities involve generating meaning rather than rules. In 'The Backward Design Process', the course is based on need-based and competency based. Like 'The Forward Design Process', 'The Backward Design Process' is based on a linear progression where the content is pre-determined prior to the delivery of courses.

English for Science and Technology (EST)

English for Science and Technology (EST) is part of language for specific purpose movement where English language is delivered keeping the specific needs of the science and technology students. English for Specific Purposes (ESP) is another synonymous term used. As per Hutchinson and Waters (1987), ESP courses are 'need-based' and what makes it different from English for general Purposes (EGP) courses is the 'awareness of needs'. Being adult learners, EST students are aware of their language needs.

Implications for language teachers and students

The role of teacher has been undergone a tremendous change. Teachers are expected to perform many other duties apart from transacting knowledge. Apart from an instructor, model and explainer, teachers need to prepare themselves for other roles. One of the key roles of a teacher is be a 'negotiator' who should consistently negotiate in the process of learning. Further, teachers need to ensure that learners express themselves and develop a sense of autonomy.

The role of students has also changed. It is not just learning which is important, but 'learning how to learn' has larger significant. Learning should be a fun activity which can be achieved through 'negotiation' and 'experiment'. Further,

EST learners being adult learners must take the onus of their own learning. The learners must involve themselves actively and practice language both inside and outside classroom.

CONCLUSION

It can be observed that there are various approaches to language syllabus design. It includes process approaches; The Forward, The Central and The Backward as proposed by Richards (2013). It is not feasible to decide that which is the best and suitable for EST students as the needs of learners vary from time to time. It is up to the teachers to decide which approach suits the needs of his/her students. An eclectic approach can also be experimented where components from all the approaches can be taken.

The following factors need to be considered before deciding which approach to be undertaken.

- Learners' academic and professional language needs
- Learners' learning strategies and motivation
- Teachers' language proficiency
- Assessment and evaluation process

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Figure 2. The Forward Design Process

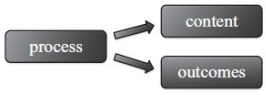

Figure 3. The Central Design Process

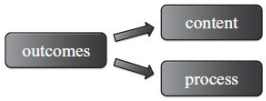

Figure 4. The Backward Design Process

Adopted from Richards (2013)

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RESEARCH ARTICLE

Modelling and Simulation of Solar Tree for Domestic Lightning Purpose

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ABSTRACT

The present research aims for modelling and simulation of solar tree which is installed in a pole mounting structure. Solar tree is an alternative method to flat type of roof mounting structure which requires more space. As per latitude of Bhubaneswar location (20^0 N), it was faced towards south and installed near Traffic side. The simulation of pole mounting structure was carried out and maximum deformation and stress were calculated. It is used for domestic lightning purpose during night time. The material of mounting structure was taken as stainless steel and main components are Solar PV panel, charge controller, battery.

Keywords : Solar Tree, pole mounting structure, maximum deformation, maximum equivalent (Von-mises) stress

INTRODUCTION

D.M.Patil et al [1] developed a solar tree which was an alternative for roof top mounting structure. This was used for domestic purpose and by using tracking system the performance was also increased. B.Ayneendra et al [2] designed a solar tree with a proper sizing of PV panel, battery, and charge controller and to increase the performance. H.Khan et al [3] developed a solar tree which uses a pole mounting structure whose main objective is to reduce the land area and to use efficiently. S.S Awaze et al [4] designed a solar tree which consists of number of solar panel integrated in a same pole mounts and installed at the site of traffic. A.P.Srinivas [5] developed a solar which consists of numbers of solar panel connected in series and parallel to generate electricity and supplied power to CFL lamp of 5 Watt. V. Avdic et al [6] designed a solar tree by using CAD software for which was a solution for urban use.

Photovoltaic Mounting Structure

The mounting structures are classified as Ground mounting structure and Roof mounting structure. Again ground mounting structures are classified as pole mounts, foundation mounts and ballasted footing mounts which does not require any excavation. Flat roof solar installation requires the three techniques such as Ballasts or weight, mechanical attachment and Hybrid mounts. Ballasts technique is used in low wind zone. Mounting Rack materials such as Aluminium and stainless steels are used due to their strength and corrosion resistance. These are the following steps for installation of mounting structure.

- Solar Panel direction should be tilted at around 15-20 degree and faced toward South for receiving maximum solar energy.
- Module Stand Model (rooftop base model) is being used here EWDS (Early Warning Dissemination System)
- Rooftop tower foundation :
- Find suitable place where no shadows from Tree or Poles.
- Clean this place and mark the base of mounting pedestal.
- Drill up to proper depth and clean the dusts.
- Put Anchor Fastener Bolt and hammer it little bit; Tighten the nuts
- Put a Square frame of height 50-100 mm.
- Mold it with grouting cement and water mix.
- Demold after 1-2 hours. Structure is ready.

Design and Simulation of Solar Tree

- Figure 2 consists of Pole mounting structure having almost 12 ft and made up of stainless steel. There were 10 numbers of head capped with photo voltaic panel (Mono/Poly), are supported by poles 0.3-0.4 ft/3.6-4.8 inch in diameter. 5 white LEDs of 10 W (1200 lm) each are situated at the bottom part of 5 of these heads and extra power can be connected to other sources.
- The base is made of reinforced concrete.
- Figure 2 shows the Ansys simulation of Pole type structure by 10 Kg load where we got directional deformation, total deformation and stress developed on the structure. The maximum directional deformation was found in x axis as 2.3622×10^{-6} mm , the maximum total deformation as 8.759×10^{-5} mm, and maximum equivalent (Von-mises) stress developed as 0.1013 MPa.
- In the Figure (3), 15 Kg load was applied on the top of the pole and total deformation was found as 4.6782×10^{-4} mm.

Solar Panels

- System Design: 12V
- Peak power of each panel: 20W

Expected Budget (INR)

- Solar Panel (20 W, Mono/Poly)- 10x1,200 = Rs.12,000
- Charge Controller (12/24V 15A) - 1x1, 200 = Rs. 1,200
- Solar Battery (12 V 80 Ah) - 1x7, 000 = Rs. 7,000
- Electrical Wires & Switches - = Rs. 500
- SS/MS Poles - = Rs. 6,000
- Civil Work - = Rs. 1,800
- Labour Charge - = Rs.

Total - Rs. 28,500

CONCLUSION

The present research describes the design and simulation of solar tree which uses a pole mounting structure and reduces space as in the flat type of structure. It will be placed near by side of the traffic area and used as lighting and also for decorative purpose during the night time. The maximum deformation and stress of pole mounting structure was found by simulation through Ansys software.

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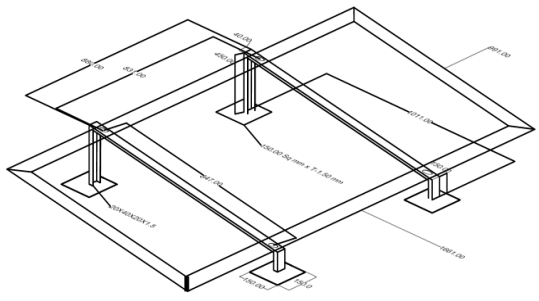

Figure 1 shows module stand made up of concrete .The dimension was specified in the figure.

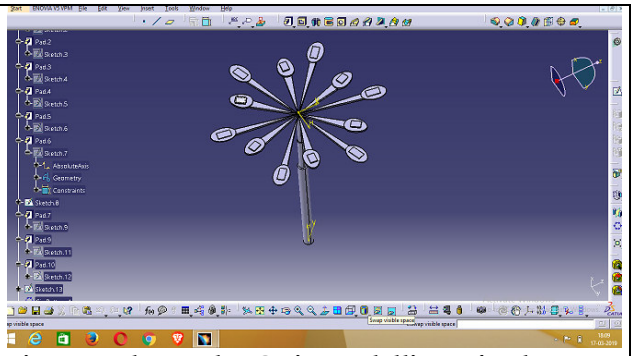

Figure 2 shows the Catia modelling of solar Tree with pole mounting structure

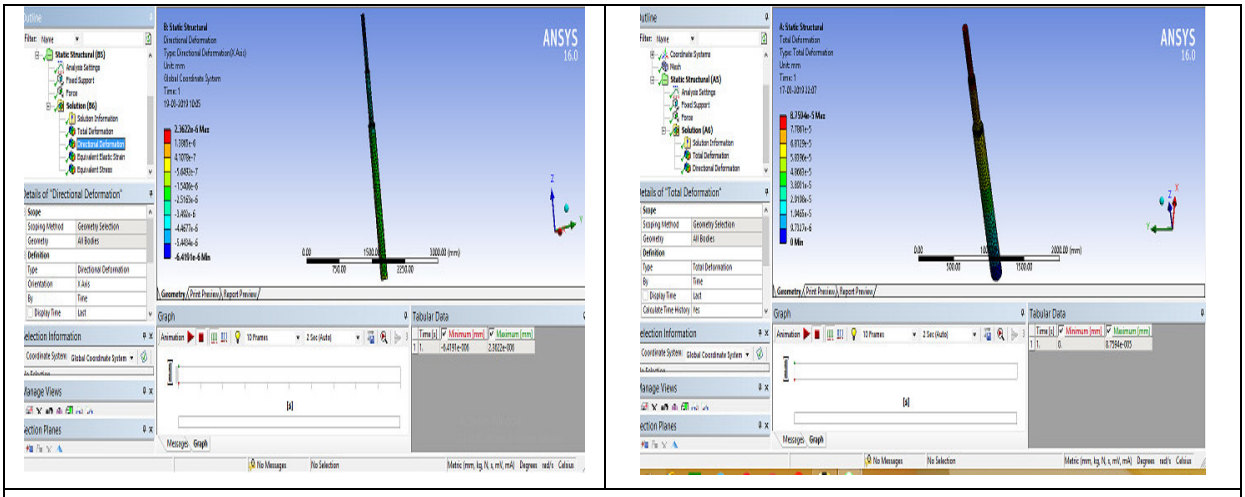

Figure 2 shows Ansys simulation of Pole type structure by taking 10 Kg load

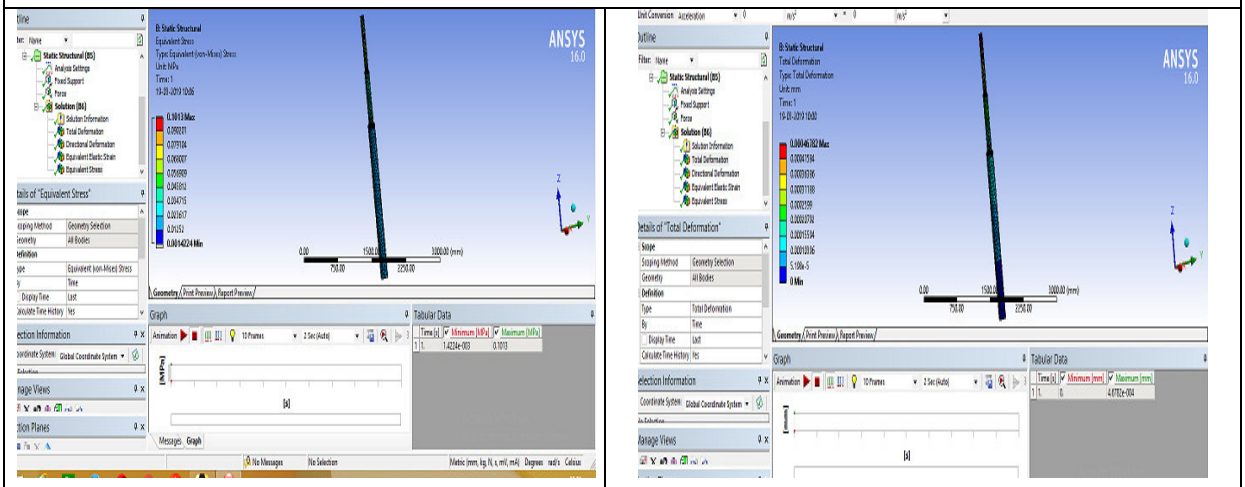

Figure 3 shows Ansys simulation of pole type structure by taking 15 Kg load

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REVIEW ARTICLE

Antimicrobial, Antioxidative and Ethnomedicinal Properties of Some Medicinal Plants of Odisha, India: A Review

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ABSTRACT

From ancient era, herbal medicine portrays one of the most important fields of traditional drugs all over the world. Medicinal plant species play a vital role to protect the life of human beings. The knowledge about curing properties has been imparted over the centuries within and between human communities. Plant kingdom produced a huge amount of biologically active and curative potentially active components. So to collect basic data many ethnobotanical surveys were attempted all over the world. Mostly plant species shows varieties of medicinal and healing properties of various diseases like bronchitis, ulcer, diarrhea, dysentery, urinary and skin disorders, etc. The species of plants is endowed with immune-modulatory, antiulcer, anticancer, antimicrobial, antitumor, antioxidant, insecticidal and herbicidal activities etc. Currently, infection caused by microbes like bacteria, virus and fungi have risen enormously and the resistance of antibiotics has become a global concern. With a hope on mind to get new drugs from the plant extracts, a special attention has been paid on this topic. To encourage the use of herbal medicine and to identify their potentiality as the sources for drugs, it is more necessary to study on indigenous plants. Like that Plant species also have natural antioxidants and produce capacity of several antioxidative components. Based on antioxidant drug formulation are used for prevention and treatment of many complex diseases. Thus in the present work reviewed the literature based on ethnobotanical studies, antimicrobial activities, antioxidant activities of plants of diversity. The study is focused on documenting the knowledge about the vegetation of the diversity and to provide future opportunities to use the flora.

Keywords: Antioxidative, Antimicrobial, Drugs, Ethnobotanical, Traditional

INTRODUCTION

Since the beginning of human civilization, medicinal plants have been used by mankind for its curative value. Nature has been a source of medicinal agents for thousands of years and magnificent numbers of contemporary drugs have been isolated from natural sources. Most of these segregations were found on the uses of the agents in traditional medicine. Jain, 1968 reported that, India has various traditional medical systems, such as Ayurveda and Unani, which has persisted through more than 300 years, mainly using plant-based drugs. The materiamedica of these systems contains a rich heritage of primordial herbal practices that helped to assist the health of many rural people of India. The ancient manuscripts like Rig Veda (4500-1600 BC) and Atharva Veda point out the utilization of various plants as medicine. The books on Ayurvedic medicine such as CharakaSamhita and SusrutaSamhita refer to use of more than 700 herbs.

UNESCO, 1996, found the application of conventional medicines and medicinal plants in many developing countries as therapeutic agents for the maintenance of good health. According to the report of UNESCO,1998 moreover, an increasing reliance on the use of medicinal plants in the industrialized societies has been detected to the extraction and development of drugs and chemotherapeutics from these plants as well as traditionally used herbal remedies. Lucy and Edgar, 1999 reported that modern pharmacopoeia still contains at least 25% drugs obtained from plants and many others which are synthetic analogues create on prototype compounds isolated from plants. Nascimento et al., 2000 characterized that such plants ought to be investigated to more readily comprehend their properties, security and strength. Kala, 2000 examined that, again in light of the fact that database on the utilization of plant species for corrective reason has been passed starting with one age then onto the next through oral custom, this information on restorative plants has started to decrease and become obsolete through the lack of ID by more youthful ages because of a move in disposition and constant financial changes.

Nautiyal et al., 2002 they considered that prompt rising interest of plant-based medications is sadly making overwhelming weight on some chose high-esteem therapeutic plant populaces in the wild due to over-collecting. A few of these therapeutic plants species have moderate development rates, low populace densities, and tight geographic extents and Jablonski, 2004 detailed that they are progressively inclined to annihilation.

Joshi et al 2004, they explored that since past decade, there has been an advanced of interest in the study of natural products are the reservoir of potential drug substance. In India approximately 85% discovery of new compounds of medicinal action is so effective from plant based sources. The three traditional medicinal systems of India, namely Ayurveda, Siddha and Homeopathy depend Homeopathy depend completely on plants for conventional formulations. World Health Organization (WHO) has calculated total international herbal drug marker as US $62 billion and is likely to rise to US$ 5 trillion around the year 2050. They also found that in India, Ayurveda alone accounts for Rs3500 cores (US$ 813 million) to the internal market annually. The worth of medicinal plants based trade in India has been calculated as Rs5000 cores per annum and is expanding yearly at the rate of 7.15. This is a manifestation of a possible raising demand for plant based drugs in near future. Approximately 90% of medicinal plants used for the formulation of conventional medicines by industries are collected together from wild in an injurious way.

Rout et al., 2005 they broadcasted from the study that 21 medicinal species in the overwood, 35 species in the middle storey, 17 species in the ground flora and 16 species of climbers, representing 38 families of families of vascular plants. Community-based conservation and management strategies can provide in solving problems related to over-exploitation and degradation of medicinal plant resources in India. Uniyal et al., 2006 they characterized that all pieces of the therapeutic plants are gathered by nearby and society networks everywhere throughout the world for their utilization however these are typically gathered in low amounts. Kala et al., 2006 additionally, he found the indigenous information on the utilization of lesser-realized therapeutic plants is likewise quickly declining. Ceaseless disintegration the in the customary information on most significant plants for medication before and the recharging interest as of late, the need existed to survey the important information with desire for building up the restorative plants division. Sandeep Pandey, 2007 analyzed on the chemical composition, ecological adaptation,

pharmacological, nutritional and ethno botanical importance of *Ocimum gratissimum* L to explore its numerous curative applications. He found that the plant is generally antimicrobial, antidiabetic, antidiarrheal, antiurilithiatic, antioxidant, antimutagenic insecticidal and anti-cancerous in nature. Okigbo et al., 2008 studied that medicinal plants are plant containing inherent active ingredients used to cure disease or relieve pain. Ncube et al., 2008 they studied that, nature has been the origin of the curative agents since ancient times. Herbal medicines have collected notable reputation worldwide due to their side effects.

Uprety et al., 2010, they were documented 56 plant species from 60 medicinal formulations, in Nepal. A 90% resemblance was reported between local plant use and found plant chemical composition and pharmacological properties for the 30 species for which data was available. Sixteen medicinal plants were ranked as priority species, 13 of which having also been prioritized in a country-wide governmental classification. Kumar and Satapathy, 2011 they recorded 72 plant species, few of which are herbs and shrubs, with some climbers, mainly belonging to class Dicotyledons. The leaves, seeds, and roots from 20, 4 and 8 plant species are used for treatments. Further the plants were observed to be highly valuable for medicinal uses including dysentery, leprosy, paralysis, piles, diarrhea etc. Anbarashan et al., 2011 conducted a survey in order to explore the medical values of scared groves in Pudukottai District, Tamilnadu. They documented a total 89species of medicinal plants belongs to 51 families. They used the medicinal plants against several diseases like throat infection, diarrhea, skin diseases, tumor, diabetes and cold, cough.

S.C. Sahu and N. K. Dhal, 2012 found that out of 57 tree species, five species were differently dispersed and 52 species were adjacently circulated. The investigation admits pervasive bunching nature of tree species in the tropical woodland of Malyagiri slope ranges. Singh et al., 2012 during the study they found that 66 therapeutic plant species having a place with 37 families and 60 genera has been archived. These plants were utilized to treat various sicknesses and aliments assembled under 11 illness classifications, with the most elevated number of species (41) being utilized for gastro-intestinal turmoil, trailed by dermatological clutters (34). Uprety et al., 2012 they introduced a survey of conventional employments of restorative plants by the Aboriginal individuals of the whole Canadian boreal woods so as to give broad documentation, perceive look into holes, and propose viewpoints for future research. An aggregate sum of 546 restorative plants taxa were utilized to treat 28 sicknesses and turmoil classifications, with the most noteworthy number of species being utilized for musculoskeletal disarranges, gastro-inside clutters. Ajibesin et al., 2012 detailed that individuals of River State, Nigeria were utilized roughly 188 restorative plant species having a place with 169 genera and 82 families to recuperate the sicknesses like dermal or stomach related issues and fever/intestinal sickness.

An ethno botanical survey of medicinal plants used in the area of Aravalli hill range was carried out by Sharma and Kumar, 2013. They have been documented 29 medicinal plant species which are used for cosmetics purpose by the tribes of this area. These plant species used by the people for curing common beauty problems like skin management and hair management. Kalaskar G M &Surana S J, 2014 they reported on 124 medicinal plant species from which 53 families were found to be used against jaundice and liver diseases by the tribal's and traditional healers. Panda et al., 2014 they reported that maximum number of sacred groves from Koraput, where only few scientific documentation of plant species in them. They documented floral diversity and uses of 94 scared plant species distributed in 63 genera be owned to 43 different families from 6 different sacred groves in a systematic manner. Panda et al., 2014 they explored the curative values of common weeds present in the crop fields, and different places like paddy field, crop field of vegetable and other localities of Koraput district (Odisha). As the result of the survey a total amount of 33 plant species belonging to 32 genera and 20 families were identified as being used for treatment of about 36 aliments including headache, toothache and eye inflammations.Patra et al., 2014 surveyed on the tribal people of Mohana region of Gajapati district, Odisha, India and the 73 plant species having medicinal properties used against asthma, breast cancer, jaundice, piles, diabetes, rheumatism, stomach disorder and skin diseases.

Satapathy, 2015 from the field examines did in Jajpur area of Odisha for recent years (1990-2010) summed up that among 1000species of blooming plants and greeneries from the region around 530 species have therapeudic esteem. Kumar and Jnanesha, 2015 learned about the restorative plants which are jeopardized requirement for earnest

security and protection. So preservation and development of uncommon and imperiled restorative harvests can be treated as an elective salary age hotspot for the rustic jobless without hampering their continuous pay creating exercises. Madharia and Jahan, 2015, they examined that in the midst of the plant decent variety not many of the plants can possibly treat numerous ailments which are alluded to as restorative plants. Hardly any chose general restorative plants utilized between the hotspot of Chhattisgarh in Traditional/Alternative remedial practice were assessed. The ethno herbal database fills in as a base for new mixes with dynamic standards for phytochemical, pharmacognostical, pharmacological and clinical research. Along these lines, upkeep of undermined plants is should be tended to direly. Kankara et al., 2015, they led an ethno plant overview to record restorative plants utilized for customary maternal social insurance in Katsina State, Nigeria, around 101 genera dispersed among 50 families were found to fix ailments like migraine, maritime torment, baby blues drain, and baby blues wound relieving had the most elevated Informant Consensus Factor (ICF) of 1.00 each. Greatest plants (68.47%) were herbs and bushes and about 84.68% of the revealed plants were wild. Leaves were for the most part utilized (32.14%) plant's part.

Pradhan et al., 2016, they currently studied betrays 91 various plant species belonging to 46 families were therapeutically used by the indigenous people. The local people mostly used these plants to heal several diseases like diarrhea, dysentery, indigestion, headache, worm infection, wound healing, stomach disorders, snake bite, Rheumatic disorder, menstrual problem etc. This will encourage a practical use of botanicals and must be continued focusing on its pharmacological validation. Xego et al., 2016 they analyzed the results show that hydroponics has the ability to develop plant growth and yield of desired plant parts even in areas where these plants do not normally grow under natural conditions. This was the case with *Siphonochilus aethiopicus.* Kumar et al., 2016 reported folk medicinal uses of approximately 26 indigenous plants among the people of villages of Manipur, which were used for aliments related to microbial diseases.

D Das and P Ghosh, 2017, they studied 30 important medicinal plant species of Southwest Bengal, India with their medicinal uses and ecological perspectives. Swagatika Patra and Pinaki Samal, 2018 they found the systematic conservation, multiplication and large scale cultivation of medicinal plants became a global concern. They analyzed of several publications and provide a widespread knowledge about the usage of plants and their parts for the treatment of several diseases in India. ShyamSundar Manna and Satyendra Prasad Mishra, 2018 they summarized that the paper, aims have been made enlist the ethno medicinal plants of Lalgrah forest range of India. The study broadcasts that 52 different plants species are used by native people to heal different diseases. Out of the 52 plant species, 17 are herbs, 20 tress 11 shrubs, and 4 are climbers. The list of plant parts, habit, mode of their use and purpose has been documented in this study.

Kumar S et al., 2018 they highlighted the use of local flora, explore, identification, ethno botany and conservation of wild and cultivated plant species in the city of Rourkela, Odisha, India. A total of 154 plant species, be owned by 128 genera and 55 families, were identified. The documentation of all useful floras with ethno medicinal potential is helpful in conserving plant biodiversity as well as in environmental surveys along with potential applications in drug discovery and oriental medicine. Axiotis et al., 2018 gave an account about the therapeutic purposes and galenic preparation by local medical doctors and pharmacists of the area of Greek islands of the North Aegean Region. They found that about 109 wild plants from 52 families, which are being used for the curative purposes. In semi-pastoral Gujjar tribe in the high altitude of Chamba, of Western Himalaya an ethno botanical survey on medicinal plants were carried out by Rana et al., 2019. They have been documented 83 plants belonging to 75 genera and 49 families that were observed to have ethno medicinal uses followed by food, household uses, fruits, and fodder.

Antimicrobial activity

From 2000 years antimicrobial use has been common in people. Ancient Egyptians and ancient Greeks used specific molds and plant extracts to heal infection. Antimicrobial activity refers to the process of killing or inhibiting the disease causing microbes or to stop their growth. Different antimicrobial agents are used for this purpose. On the basis of microorganisms antimicrobial medicines can be categorized. It may be antibacterial, antifungal and antiviral.

For example, antibiotics are used against bacteria, antifungal are used against fungi and antiviral are used against virus. They all have different modes of action by which they act to suppress the infection. Rios and Recio, 2005 recorded the detailed data of such as history of uses of medicinal plant, future aspects of medicinal plants and the current status of medicinal plants on the basis of potential antimicrobial properties and also as a source for natural compounds that act as new anti-infection agents. They documented the number of published articles based on the antimicrobial activity of medicinal plants in PubMed. During the duration between 1966 and 1994, they found about 115 articles, after then from 1995 to 2004 they found 307 articles.

Dabur et al., 2007 worked with 77 extracts from 24 plants having antimicrobial properties was screened against 8 bacteria and 4 pathogenic fungi, using microbroth dilution assay. The objective of the study was to assess the antimicrobial activity of some medicinal plant used in Ayurveda and traditional medicinal system for treatment of manifestations caused by microorganisms. As result they found that antimicrobial activity of plant extract was considered to be good if its MIC was less than 100.0 µg/ml, moderate if MIC was from 100.0 to 500.0 µg/ml and poor over 500.0 µg/ml.

NCC and Junior A, 2010 carried out a scientific survey on biological characteristics of medicinal plant species and their pathogenic microorganisms resistant to antimicrobials. At the time of secondary vegetal metabolism produced active compounds which are responsible for the biological properties of certain plants used to cure various diseases like infectious diseases all over in the world. Shihabudeen et al., 2010 surveyed and gave a report on the presence of coumarins, flavanoids, glycosides, phenols, tannins, saponins and steroids. In this survey, methanol extracts of six plants, which had been explained in herbal books and folk medicine of India, were screened for their antimicrobial activity against certain pathogenic bacteria and fungi that can cause gastroenteritis, urinary tract infections, pneumonia, urinary tract, burns and wounds, lung infection and toxic shock syndrome.

Selvamohan et al., 2012 studied those seven medicinal plants (*Aloe vera, Phyllanthus emblica, Phyllanthus niruri, Cynodon dactylon, Murryakoenigii, Lawsonia inermis, Adha-thoda vasica*) which were collected from Nagercoli, Tamilnadu, India. Those have been used for therapeutic treatments which were estimated for activity against pathogenic bacteria such as *Staphylococcus sp., Escherichia coli, Klebsiella sp., Pseudomonas sp*. The invitro antimicrobial activity was performed by agar well diffusion method and disc diffusion method. The ethanolic and aqueous extracts showedminimum antimicrobial activity when compared to methanolic extracts. The methanolic extract *Phyllanthus niruri* (stone breaker) showed the maximum activity against *Staphylococcus sp.*

Alavijeh et al., 2012 described that most plant extracts produced antibacterial and antifungal properties. The present survey was instigated because of the increasing resistance to antibiotics including bacteria and fungi. Plant extracts and compounds are of new interest as antiseptics and antimicrobial agents. As result extracts of *Azadiracta indica* and *A. nilotica* recorded to control higher antimicrobial activity among the other tested medicinal herbs.

Narware et al., 2014 gave a review on the current study of antimicrobial activity and phytochemical effect of the plant *Gardenia gummifera* Linn (Rubiaceae) which is commomly known as Dikamali against some microbes like *S. aureus* and *E.coli*. Dikamli has gum pitch exudates from the leaf buds of these trees. Dikamali has various therapeutic properties which incorporate antispasmodic, carminative, anthelmintic, diaphoretic and expectorant. It is likewise professed to be helpful in dyspepsia, tooting for cleaning ulcers and wounds and to keep off flies from wounds in veterinary practice. Sree et al., 2014 gave a detailed account on the study to analysis medicinal potential of five mostly used plants such as *Naravelia zeylanica* DC., *Adhathoda zeylanica* Medic, *Cassia auriculata* L., *Vitex negundo* L., *Orthosiphon staminus*, of Western Ghats of India. Many of the extracts performed activity against pathogenic bacteria and fungi. The objective of the study was to actuate the content of total phenolics and total flavonoids and to evaluate total antioxidant activity, free radical scavenging activity, and to determine the antimicrobial activity of five Indian medicinal plants of Western Ghats. The overall antioxidant activity of *Narvelia zeylanica* and *Adathoda zeylancia* were found to be the strongest.

Farjana et al., 2014 studied that the antimicrobial activity of extracts of guava, green tea, neem and marigold against various species of bacteria. By agar well diffusion method they examined the antibacterial activity of plant extracts.

They concluded that the leaves of guava, green tea, neem and marigold show antibacterial activity against different pathogenic bacteria species. They could be used as alternatives to common antimicrobial agents for treatment of bacterial infections. Leaves and bark of the guava plant are distinguished for the cure of diarrhoea, colds, toothaches and swelling. Green tea is used for the treatment of lung, pancreas, liver, skin cancers etc. Neem leaves are used to control hepatitis, and diabetes, and marigold leaf is knows to be highly effective because of its therapeutic use against burns and bruises.

Javid et al., 2015 carried out a experimental survey to recognize the in-vitro efficacy of three medicinal plants such as *Artemisia indica*, *Medicago falcata* and *Tecoma stans* in Pakistan against selected bacterial and fungal strains. They concluded that those plants have traditional uses and also have antimicrobial properties. Antimicrobial activities may be due to strong occurrence of active compounds i.e. saponins, tannins, alkaloids, steroids, phenols and flavonoids. Packer et al., 2015 organized an ethno botanical survey with Yaegl Aboriginal community of northern New South Wales, Australia. They surveyed that the antimicrobial prpperties of plants used to cure the wounds, sores and skin infections. Aqueous or 80% aqueous ethanolic extracts from nine selected plants such as *Alocasia brisbanensis*, *Canavalia rosea*, etc. were tested against the Gram positive and Gram negative antibiotic sensitive bacteria. They concluded that Aqueous and 80% aqueous ethanolic extracts of *Lophostemon suaveolens*, *Corymbia intermedia* and *Syncarpia glomulifera* exhibited promising levels of antimicrobial activity against a range of both antibiotic sensitive and resistant strains of microorganisms This study showed the value of customary knowledge in the identification of new sources of antimicrobial treatments.

Sailaja V. et al., 2016 carried out a research on seed of six plants having medicinal properties such as *(Acacia catechu, Sida cordifolia, Momordica fotida, Albiziz procera, Mesua ferrea and Lantana camare)* for the experiment on antimicrobial activity by using 4 types of solvet like water, Acetone, Petroleum Ether and chloroform. Plants seed extracts showed highest zones of inhibition on gram positive bacteria than gram negative species. They concluded that this study may help in the future study and discover many more novel curative agents from plants. Lakshmi Sundaram, 2016 explored that the antimicrobial potential of *Messua ferrea* examined for their antibacterial effect on certain selected strains of bacteria by using the standard method of diffusion disc plates on agar and MIC was estimated using dilution method. Final result showed the antimicrobial properties of the selected plant. Erecevit and kirbag, 2017 conducted a survey to explore the antimicrobial activities of some medicinal plants. They took extracts of eight species which have therapeutic properties such as *Rhus coriaria* L., *Pistacia terebinthus* L., etc. screened against pathogenic microbes. They concluded that the extracts of *R.coriaria, P.terebinthus* subsp. *Palestina, U. erectus* and *C. virgata* reported antimicrobial activities against to bacteria, yeasts and dermatophyta. Also there was no effect of the extracts on some microbes.

Egamberdieva et al., 2017 reported that to isolate and characterize enodohytic bacteria from two medicinal plants, *H. perforatum* and *Z. capitata*, with contrasting antimicrobial activities from Chatkal Biosphere Reserve of Uzbekistan and evaluate their plant-specific traits involved in bio-control and plant growth promotion. The antagonistic isolates were able to control tomato root rot caused by *Fusarium oxysporum* and stimulated plant growth under greenhouse conditions and could thus be a cost-effective source for agro-based biological control agents. At the end indicate that further research is necessary to resolve the impact of medicinal plant species with contrasting antimicrobial activity on the endophytic microbial community in more detail, and to identify biological active compounds produced by the hosts and their endophytes.Romulo et al., 2018 surveyed that a total of 49ethanol extracts from 37 various medicinal plant species of Indonesia, belonging to 23 different families were screened for their in vitro antimicrobial activity. They concluded that leaf extract of O. aristatus and W. floribunda displayed significant anti-candidal effects. Therefore, both of these plants could serve as source materials for the development of new anti-candidal agents. However, future phytochemical research based on these species will be needed to isolate and characterize their antimicrobial effective constituents. Tlili et al., 2019 worked on seven aromatic plants which were used traditionally in the Tunisian region in folk medicine. They focused on the biochemical and biological characteristics of the taken plants. After the test all the plants sighted a phenomenal existence of secondary metabolites. R. tripartite and Z. lotus

were occurred to be especially effective in anti-proliferative activity, while *H. fontanesii* were presented to have the best anti-inflammatory activity.

Antibacterial activity

Anything that kills bacteria or muffles their growth or their capacity to reproduce is known as antibacterial activity. Heat, chemicals like chlorine, and antibiotic drugs all have antibacterial properties.Nascimento et al., 2000 reported that the antimicrobial activity of certain plants which extracts were used for the test such as *Achillea millifolium* (yarrow), *Caryophyllus aromaticus* (clove), *Syzgyum joabolanum* etc. They found the highest antimicrobial potential showed for the extracts of *Caryophyllus aromaticus* and *Syzgyum joabolanum*, which inhibited 64.2 and 57.1% of the tested microorganisms, respectively, with higher activity against antibiotic-resistant bacteria (83%). Association of antibiotics and plant extracts showed antibacterial activity against antibiotic-resistant bacteria. The results obtained with *Pseudomonas aeruginosa* was particularly interesting, since it was inhibited by clove, jambolan, pomegranate and thyme extracts. This inhibition was observed with the individual extracts and when they were used in lower concentrations with ineffective antibiotics.

Ushimaru et al., 2007 studied the antimicrobial activity of methanolic extracts of some medicinal plants against *Escherichia coli*, *Salmonella typhimurium*, *Staphylococcus aureus* and *Enterococcus* sp. They concluded that the methanolic extract of *Caryophyllus aromaticus* obtained the highest anti-*S.aureus* activity and was valuable against all bacterial strains screened.Khan et al., 2013 found a report from the current survey that the antimicrobial activity of three plants *Bergenia ciliate*, *Jasminum officinale*, and *Santalum album* screened against human pathogenic bacteria like *Escherichia coli*, *Pseudomonas aeruginosa*, *Staphylococcus aureus*, *Bacillus subtilis* and *Proteus vulgaris* by using agar well diffusion method. Amid the three extracts of plants *B. ciliate* displayed the highest activity against *B. subtilis*. Roger et al., 2015 the current study was undertaken to investigate traditional process of healing typhoid in Bamboutos division. They preferred 38 plants species for screening the antimicrobial properties. All the extracts of plant species displayed activity against pathogenic bacteria like *S. typhi*, *S. paratyphi* A and *S. paratyphi* B. The final outcome was maximum plants sample used for the treatment of typhoid as anti-typhoid drugs.

Stankovic et al., 2016 reported the antibacterial activities and antioxidant capacity of eight aromatic plants, which are used as drugs in the region of the Balkan Peninsula. They took the plants such as *Hyssopus officinalis*, *Angelica pancicii*, *Tanacetum parthenium* etc, against 16 pathogenic bacteria like *E. coli, P. aeruginosa, S. pyogenes* etc. They concluded that *A.crithmifolia, A. grandiflia and A. absinthium* had maximum antioxidant characteristics while *A. sylvestrys, L. latifolium* showed the minimum probable. A phytopharmacological survey by Surrbar et al., 2017 revealed that *Ricinus communis* leaves extracts are used to cure candidiasis, skin and wound infections in Ghana. They found that aqueous, methanol and ethanol extracts were exposed to have most of the phytochemicals analyzed. As result methanol extract displayed highest antimicrobial activity and petroleum ether showed lowest antimicrobial activity. Also this survey will help in further study on antibacterial and antifungal activity of the plant.

Masoko, 2017 evaluated from the survey that *Spilanthes mauritiana* crude extracts tested against pathogenic bacteria for biological activity. They concluded that current study displayed the presence of compounds in S. mauritiana against tested pathogenic bacteria. Bereksi et al., 2018 took a survey and investigated that the antibacterial activity of extracts of certain plants like *Cassia angustifolia, Cistus monspeliensis* and *Nigella sativa* screened against various types of gram strains bacteria. Result of this study signified that the antibacterial activity supports their use to heal the infectious bacteria.

Antifungal Activity

Demolishing fungi or reducing their growth rate is known as antifungal activity. Saha D et al., 2005 reported that ethanol and aqueous extracts of 30 plants from sub- Himalaya West Bengal (India) used for controlling four foremost foliar fungal diseases of tea were screened against the pathogenic microbes. Among all the samples, extracts of *Allium sativum* L., *Datura metel* L., *A. joss*, and *Curcuma longa* L. documented 100% inhibition of spore germination. As result the antifungal compound from those plants may be used in controlling the fungicides for tea.

Dellavalle et al., 2010 surveyed and provide the details on the antifungal properties of extracts of 10 plant species used in conventional Uruguayan medicine against the phytopathogenic fungus Alternaria spp. In the midst of 29 evaluated extracts, 31% of the extracts reduced the growth and also three solvents were examined on different tissues of the plants. Acid extracts of the plants were more valuable than the aqueous or buffer extracts against Alternaria spp. equivalent to principles acquired with the traditional fungicide captan. The extracts of *Salvia sclarea, S. officinalis* and *R. officinalis* could be regarded as potential sources of antifungal compounds for healing diseases in plants. These extracts displayed highest activity, still at very least concentrations, and the equal fungicide effects as chemical fungicide. They finish with the conclusion was that extracts of plant samples reveal incredible fungicidal characteristics that maintain their conventional use as antiseptics.

Ambikapathy et al., 2011 observed the antifungal activity of five special medicinal plants extracts such *as Lawsonia inermis* L., *Mimosa pudica* L., *Tephrosia purpurea* , and *Vinca rosea* L. were screened against pathogenic fungi like *Pythium debaryanum* by using the method of agar well diffusion. Among the three solvents like n-butanol, methanol and aqueous, the methanoloc extracts of *L. inermis* displayed highest amount of antifungal properties against *P. debaryanum*. Masih et al., 2014 regarding the enormous prospectively of plant as sources for antimicrobial drugs with reference to antibacterial and antifungal agents, a systematic investigation was carry out to test the local flora for antifungal activity from the leaves extract of *Pongamia pinnata*, *Calotropis procera*, *Nerium indicum* and *Curcuma longa* were taken in aqueous solution, screened against pathogenic microbes- *Aspergillus fumigatus*, *Alternaria solani*, *Helminthosporium* spp. and *Fusarium solani*. As final result they found that aqueous extracts of *Calotropis procera* leave was a good source of antimicrobial components and also the latex of plants had a property of spectrum antifungal activity and plants used in the treatment of infectious diseases.

Silva et al., 2014 observed that to identify the competence of aqueous extracts from medicinal plants against the pathogenic organisms of coffee tree. Extracts of plants from different parts like bulbs of *A. sativum*, flower buds of *S. aromaticum*, leaves of *V. polysphaera*, *Azadirachta indica, Ricinus communis* and *Cymbopogon citratus* screened against pathogenic fungus such as *Cercospora coffeicola, Fusarium oxysporum, Phoma tarda* and *Hemileia vastatrix*. Experiments carried out in vitro conditions based on mycelia growth and conidial germination inhibition. The mainly valuable plan extracts against the micellial growth and conidial germination were *V. polysphaera*, *S. aromaticum* and *A. sativum*. Abkhoo and Jahani, 2016 surveyed and noticed that the antifungal activity of the medicinal plant species, collected from Sistan region, Iran like *Peganum harmala, Glycyrrhiza glabra, Mentha spicata* and *Rosmarinus officinalis* which were used as conventional medicine tested against pathogenic microbes like *F. oxysporum*. It showed the result that out of total herbal extracts four displayed fungistatic activities and two presented fungicidal activities. At final stage of research they found antiungal activities of herbal medicines against *F. oxyspoum*. Especially extracts of *G. glabra* showed bioactive components effectual to reduce the growth of *F. oxysporum.*

Salhi et al., 2017 documented the detailed that the antifungal properties of aqueous extracts from native plants such as Artemisia *Herba alba, Cotula cinerea, Asphodelus tenuifolius* and *Euphorbia guyoniana* that grow instinctively in the Northern Sahara of Algeria screened against two fungal species of *Fusarium* genus in in-vitro assay. The final result attained that the antifungal activities of *C. cinerea*, *A. tenuifolius*, and *E. guyoniana* used for manage the fungi affecting wheat yield safely. Also it evaluated the use of extracts as Integrated Pest Management. Santos and Pereira, 2018 enlisted 38 plants of Candida species having medicinal properties were used by the Brazilian people for conventional purpose against pathogenic micro organisms. Survey had also disclosed that the plants examined were not toxic at curative doses with good antimicrobial properties. They concluded plant extracts used to produce developed phytomedicine to heal oral candidiasis for multi resistant Candida albicans.

Antioxidant Activity

Antioxidant activity is described as a confinement of the oxidation of proteins, lipids, DNA or different particles that happens by obstructing the spread stage in oxidative chain responses and essential cancer prevention agents legitimately rummage free radicals, while auxiliary cancer prevention agents by implication forestall the arrangement of free radicals through Fenton's response. Cell reinforcements movement is an uncommon case of a

useful preferred position that plant concentrates can convey. Plants are recognized to have a scope of normal cancer prevention agents that shield and save their physical and metabolic trustworthiness just as their heredity by method of their seeds. The vast majority of these concentrates and parts from plants are ascending as contender for sensible the impacts of the maturing procedure on skin by constraining biochemical results of oxidation. In other word cell reinforcement is a substance that decrease harm as a result of oxygen, for example, that brought about by free radicals. It might assume an imperative job in coronary illness, malignant growth and different infections. Cancer prevention agents, similar to Vitamin and E and carotenoids may help protect cells from harm brought about by free radicals. Other normally happening cancer prevention agents incorporate flavonoids, tannins, phenols and lignans. Plant based nourishments are the best sources. These incorporate organic products, vegetables, entire grains, nuts, seeds, herbs and flavors.

Gacche and Dhole , 2006 took a survey to investigate that 50% alchol extracts of different parts of some selected plant species such as *Swertia chirayita, Cedrus deodar, Pongamia glabra* etc. were tested for antioxidant and anti-inflammatory potential. Selected plants under the survey were showed to be efficient scavengers of DPPH radicals. Finally they concluded that it will help in the further study and use for standardization and validation of traditional medicines containing active components.Harnafi and Amrani , 2008 enlisted all the data from the reviews that the foremost important colorimetric techniques used to find out polyphenol content in extracts of medicinal plant species and the spectro photometric assays utilized to assess their antioxidant power.

Mosquera et al., 2009 reported for the first time on the antioxidant activity of Colombian species. They surveyed the antioxidant properties of methanol extracts of forty-six plants, belongs to the families Asteraceae, Euphorbiaceae, Melastomataceae, Rubiaceae and Solanaceae, collected from Regional Natural Park, Colombia. Among all the extracts *Phyllanthus sp., Tibouchina grossa, Miconia lehmannii* and *Lycianthes radiate* were displayed the maximum antioxidant activity 54%, 47%, 45.3% and 41.5% respectively.

Jaber et al., 2011 described plant extracts and their compounds present in foods and medicinal plants as a natural source of antioxidants have been comprehensively analyzed. Objective of the survey was to find valuable antioxidants for the cure purpose or control of free radical- mediated deleterious effects. Krishnaiah et al., 2011 studied that natural antioxidants stand for a prospective side effect- free substitute to synthetic antioxidants in the food processing industry and for use in defensive medicine. The aim of the study was to record medicinally magnificent plant species from around the world and displayed that many have high antioxidant activity when compared to synthetic antioxidants. Ho et al., 2012 noticed form the study was to test the probable antioxidant activities of the methanol and water extracts of 31 medicinal plants in Taiwan. They found that *Rotala rotundifolia*, *Juncus effusus* var. *decipiens*, *Cyperus iria*, *Salix warburgii*, *Lindernia antipoda*, *Kyllinga brevifolia*, and *Typha orientalis* acquired both high antioxidant activities and high amount polyphenol contents. From the results established that antioxidant activities were not directly related to polyphenol quantity. So, phytochemicals will play a vital role in the potent antioxidant activity of wetland medicinal species.

Chirag et al., 2013 presented a special note on the variety and vast potential applications of antioxidant or free radical manipulations in control and cure of diseases. Natural products from dietary compounds like Indian species and medicinal plants are known to acquire antioxidant activity. Objective of the study was to display the antioxidant/ antiradicals and their function in human body and also their presence in spices and herbs. In amplifying intake of dietary antioxidants may help to sustain an adequate antioxidant status. To defend the cells and organ systems of the body against reactive oxygen species, humans have progressed a highly sophisticated and complex antioxidant protection system. Rayasandra et al., 2013 evaluated of antioxidant properties of extracts of various type of medicinal plants and their association with the total phenolic contents (TPCs). They tested 35 medicinal plants from which four plants were chose for the experiment. The methanol extracts of *Acacia catechu* (AC-ME), *Adenanthera pavonia* (AP-ME), *Holopetelea integrifolia* (HI- MI) and ethanol extacts of *Terminalia paniculata* (TP-EE) displayed maximum antioxidant activity with 50% inhibitory concentration. In the end plants could serve as a natural source of antioxidants in the food industry and with their other pharmacological properties.

Proestos et al., 2013 surveyed on the characterization and qualification of the phenolic fraction of some selected aromatic plant extracts and essential olis collected from Greece, their antioxidant activity evaluation, and estimation of essential oils by specific assays. As result the methanolic solutions of the essential oils displayed maximum antioxidant properties. Thus it concluded that the screened aromatic plants contain some specific quantities of polyphenols and flavonoids, which are perfect sources of antioxidants.

CONCLUSION

The above review showed therapeutically properties of plant species all over the world and displayed that many have high antimicrobial activity and antioxidant activity. Most of the drugs used in the area are prepared from fresh plants collected the wild. The plant parts such as bark, flowers, rhizomes, roots, leaves, seeds, gum and sometimes whole plant were used for the medicinal purpose. Among them many of the plant species have high phenolic content and a large quantity of flavonoids, tannins, lignin and flavonols. Special attentions on plants have different families from around the world to understand and to record the curative uses and antioxidant activities. The new findings and the detailed knowledge these medicinal plants possess antioxidant and curative properties entails that making these plants as an integral part of daily consumption may control several diseases. Several types of studied on the mechanism of action, interactions with other medicinal plants or components, and the extracts should be given high attention. Current survey found that the antibacterial activity vary with the species of plant and parts of plant. So it proved that antibacterial activity could be the potential source for the discovery of new herbal medicine. Recently the World Health Organization (2002) promotes and recommends herbal medicines in national health care programs. So, medicinal plants improve the socio economic situations as well as lives of tribal. The curative uses of plants used for healing several diseases include cold, cough, jaundice, diabetic, skin diseases and cancer etc.

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Table 1. List of plants and their antioidative activity

Sl. No.	Name of the Plant species	Family	Parts used	Name of the Solvent	Antioxidant activity test method	References	Year
1.	*Alchemilla persica*	Rosaceae	Aerial parts and root	Methanol	1,1-diphenyl-2-picrylhydrazyl (DPPH)	Acikara et al.,	2010
2.	*Terminalia chebula*	Combretaceae	Fruits	Polyphenolic	DPPH	Saha and Verma	2014
3.	*Melia azedarach*	Meliaceae	Root bark	Polyphenolic	DPPH	Nigam and Sodhi	2014
4.	*Ocimum sanctum*	Lamiaceae	Leaf	Aqueous	DPPH	Nigam and Sodhi	2014
5.	*Rhizophora mangle*	Rhizophoraceae	bark	Polyphenols,	DPPH	Rashed	2014
6.	*Ligustrum vulgare*	Oleaceae	Leaves		DPPH	Rashed	2014
7.	*Anethum graveolens*	Apiaceae	Flowers	Ethanolic	DPPH	Haghju and Almasi	2015

8.	*Coriandrum sativum*	Umbelliferae	Seed	Aqueous	DPPH	Haghju and Almasi	2015
9.	*Combretum apiculatum*	Combertaceae	Leaf	EtOH	DPPH	Lawal et al.,	2016
10.	*Telfaria occidentalis*	Combertaceae	Leaf/ Root	MeOH	DPPH	Lawal et al.,	2016
11.	*Acalypha racemosa*	Euphorbiaceae	Leaf/ Stem	MeOH	DPPH/NO/OH	Lawal et al.,	2016
12.	*Garcinia lucida*	Clusiaceae	Fruit/ Bark	MeOH	DPPH, NO, OH	Lawal et al.,	2016
13.	*Spilanthes mauritiana*	Asteraceae	Whole plant	Acetone/ Methanol	Microbroth dilution assay & bioautography	Masoko	2017
14.	*Curcuma longa*	Zingiberaceae	Rhizome	Aqueous	Phospo-molybdenum	Puspal et al.,	2018
15.	*Piper betle*	Piperaceae	Leave	Aqueous	Phospo-molybdenum	Puspal et al.,	2018
16.	*Rhus natalensis*	Fabaceae	Root bark	Aqueous	DPPH	Kimondo et al.,	2019
17.	*Acacia nilotic*	Fabaceae	Stem bark	Aqueous	DPPH	Kimondo et al.,	2019
18.	*Pappea capensis*	Sapindaceae	Stem bark	Aqueous	DPPH	Kimondo et al.,	2019
19.	*Bougainvillea glabra*	Nyctaginaceae	Bark	Methanol	DPPH	Hossain et al.,	2020
20.	*Licuala grandis*	Arecaceae	Leaves	Methanol	DPPH	Hossain et al.,	2020
21.	*Anthurium crystallinum*	Araceae	leaves	Methanol	DPPH	Hossain et al.,	2020

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RESEARCH ARTICLE

Experimental Study of Solar Dish Type of Solar Concentrator

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ABSTRACT

The aim of this research is to develop a solar dish type cooker for domestic cooking purpose in rural area where there is no access of electricity and to ensure the sustainable development through clean energy. Many researchers had developed the solar dish type of cooker where the material like Aluminium was taken as glazing or polishing surface as reflector. But in this research there were number of Chromium vinyl material strips were attached on the dish which acts as reflector in order to increase the reflectivity and to enhance the efficiency. The cooking power and Energy generated for the steam was calculated as 835 W and 0.977 KW.The maximum temperatures was measured in a sunny day as 136^{0}C which is sufficient enough to cook food and for generating steam.

Keywords : Solar dish, Concentrator, Chromium vinyl, reflectivity

INTRODUCTION

Due to the maximum energy consumption in India the world energy demand is expected to rise more than 25% in next 20 years. It has been observed that industrial sector accounts more than 50% of the world energy consumption followed by transportation and building sector. Energy consumption is different for rural and urban area. Maximum energy is consumed in rural area as domestic purpose like cooking and lightning purpose. Generally the resources like cow dung, fire wood, agricultural residue are used as fuel for cooking purpose which results environment pollution and health issue.So solar operated cooking device is the alternative source for solving the problems.

M. Kumar et al [1] had done the performance testing of parabolic dish type solar cooking device .By taking the specific aperture area and focal length he had done the experiment by using different types of materials for cooking vessel. K. Schwarzer et al [2] designed an analytical method for designing simple cooking system.V.Kumar et al. [3] developed a portable dish solar cooking device which is used for frying purpose. He had designed a prototype and performance was formulated with SK 14.I.L Mohammed [4] had designed a parabolic type of dish collector by taking aperture diameter as 1.8m and focal length as 69.8 cm.The cooker was capable of cooking 30Kg of rice with in 90 to

100 minutes. S.Das. et al [5] had done the thermal analysis of parabolic type of dish cooker in which he got the thermal efficiency as 54% and at a steam rate of 0.91 kW.

Experimental set up

The main components of the solar dish type of collectors are dish type of reflector and receiver. There are number of segment of chrome vinyl material are attached in the surface of dish and act as reflector. The receiver was placed at a focal length and placed perpendicular to the centre of the dish. The dish was placed on the structure in such a way that it will be manually operated as per the direction of the sun's position. The receiver was painted as black in order to absorb maximum solar radiation. This dish having 2 m aperture diameter, 0.5 m depth and 0.3 m focal length was designed, constructed and fabricated. The receiver was made up of aluminium container and entire surface of the dish is stainless material. As the sun radiation incident on the reflecting surface of the dish, it will concentrate all the radiation into the receiver which was placed at focal distance. It will absorb the heat and gets food cooked.

Mathematical modelling

The focal distance was calculated as $f=d^2/16h$ equation 1

$$\tan\varphi = \frac{1}{\frac{d}{8h}-2h/d}$$ equation 2

Where, f=focal length, d=diameter of aperture, h=depth of parabola □= rim angle.

RESULT AND DISCUSSION

The solar cooker was put in an open atmosphere and where there was no shadow effect. With a regular interval of time the temperature reading was taken with the help of Temperature sensor and Solar irradiation was measured with the help of Lux meter. The maximum temperature reached up to 136^0C which is sufficient enough to cook the foods and also boil the water in the table 1.The amount water taken as 2 litres for testing purpose. Throughout the day a manual operated tracking device was used to rotate the dish as per the direction sun's position.

The cooking power was calculated as 835W by taking maximum interval temperature as 136^0 C and 130^0C. C_{water} =4.2J/g^0C or 4179.6J/KgK.

It has been observed that the maximum amount of water evaporated in 30 minutes is 0.65 Kg.The mass flow rate computed as 3.611×10^{-4}Kg/s. By taking latent heat of vaporisation=h_v=2706 kJ/Kg, the total energy of the steam per unit mass= $3.611\times10^{-4}\times$ 2706=0.977 KW

CONCLUSION

The present research describes about the performance testing of dish type of solar cooker. The cooking power and total energy of the steam was calculated. The amount of heat produced by the cooker was sufficient enough to cook foods. There was some heat lost to the atmosphere and again when the intensity of solar radiation decreases, there was no possibility of cook the food. Further scope of research is to reduce the heat loss and increase the cooking power.

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Figure 1 represents the experimental set up of solar dish type concentrator with manual operated tracking system

Table 1 Represents the Temperature verses time of solar dish type of cooker

Si no	Timing (AM/PM)	Temperature in 0c	solar irradiation in LUX
1	10 AM	90	71400
2	11 AM	95	71900
3	12 AM	120	72500
4	12:30PM	130	80900
5	1:00 PM	136	73600
6	2 PM	100	53600
7	2:30 PM	70	12300
8	3:00 PM	67	12000
9	3:30 PM	61	12000

Table 2 show the amount of water evaporated in regular interval of time

Si no	Timing required for boiling water in minutes	Kg of water boiled
1	30	0.1
2	60	0.25
3	90	0.45
4	120	0.5
5	150	0.65
6	180	0.7

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RESEARCH ARTICLE

Design of a Meander Line Broadband Small Antenna

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ABSTRACT

This paper presents a design of meander line broadband small antenna which is proposed for Wi-Fi applications. This antenna consists of a substrate called FR4 having relative dielectric constant 4.4, then a microstrip feedline on the ground plane and a meander line on the patch. It is designed to operate at 2.4 GHz and its whole size is 8.5 mm×8.5 mm×1.524mm. This is one of the smallest antennas available at this frequency. In this design, we used a single layer substrate ad easily simulated by high frequency structure simulator (HFSS). The simulated S_{11} plot shows that return loss is than -10 dB. The simulated radiation pattern and 3D polar gain show a positive gain which satisfies the good condition of an antenna design. The antenna performance is studied numerically. It can be a good candidate for future compact wireless devices that require a compact and simple antenna structure with a good performance.

Keywords- Meander line, return loss, radiation pattern, electrically small antenna, broadband antenna.

INTRODUCTION

Impedance band width of 50 MHz at 2.4 GHz. The various electrically small antenna is proposed in [1]. The best design has been used metallic curved strips to get better performances. The simulated results showed a 10dB impedance bandwidth of 22.4 MHz. A compact CPW-fed zeroth-order resonant antennas (Dimensions: 0.201 $\lambda 0$ × 0.17 $\lambda 0$) have been presented in [2]. By adding chip inductors to the antenna, impedance bandwidth has increased to 210 MHz. A wideband and compact antenna (Dimensions: 0.55 $\lambda 0$ × 0.55 $\lambda 0$) is proposed in [3]. The antenna consists of two arms with eight via that resonate at 3.3 GHz and had a -10dB impedance bandwidth of 220 MHz. A compact planar monopole backed antenna with a 2 × 1 array of electromagnetic bandgap structures (Dimensions: 0.31 $\lambda 0$ × 0.55 $\lambda 0$) for wearable applications has been proposed in [4]. The simulated results showed a -10dB impedance bandwidth of 120 MHz. An electrically small dipole antenna using a non-periodic left-handed transmission-line structure is presented in [5]. The 4.8% bandwidth can be obtained through optimizing the values of the series capacitors and shunt inductors. A single-layer Inductively coupled capacitively loaded monopole antenna with small ground plane for 2.362 GHz is reported in [6]. The simulated -10 dB impedance bandwidth is 0.36%. A CPW fed chip

inductor loaded electrically small antenna for WLAN frequency is proposed in [7]. To achieve a compact size and a bandwidth of 40 MHz, an open-ended coplanar transmission line has been loaded with a chip inductor. An electrically small antenna is constructed by using multiple coupled split-ring resonators (SRRs) in [8]. The proposed antenna had six layers and a relative bandwidth of less than 0.3%. In [9], it is shown how to design a compact antenna with a tuning inductor and an inductively coupled feed system. The measured results showed a -6 dB bandwidth of about 110 MHz at 2.42 GHz. One of the ways to increase the gain of electrically small antennas is to increase the area of the antenna, which is improved in [10] by antenna array. By increasing the antenna area through the array, they have been able to increase the gain from -15.4 dB to -5.5 dB.

Meanderline antenna

The design of meander line antenna is a set of horizontal and vertical lines. Combination of horizontal and vertical lines forms turns. Number of turns increase efficiency increases in case of meander line if meander spacing is increase, resonant frequency decreases. At the same meander separation increases resonant frequency decreases. A meander antenna is an extension of the basic folded antenna and frequencies much lower than resonances of a single element antenna of the equal length. Radiation efficiency of meander line antenna is good as compare to conventional half and quarter wavelength antennas. Antenna size reduction factor α depends primarily on the number of meander elements per wavelength and spacing of the element widths of the rectangular loops. The meander line element consists of vertical and horizontal line so it formed a series of sets of right angle bends. The polarization of antenna depends on radiations from the bend, the spacing between two bends is very vital, where if the bends are too close to each other, then cross coupling will be more, which affects the polarization purity of the resultant radiation pattern. In other case the spacing is limited due to the available array grid space and also the polarization of the radiated field will vary with the spacing between the bends, and the spacing between the microstrip lines. Planar meander line antenna with added quarter parasitic element at both side of the meander can produce double radiation pattern at frequencies much lower than resonances of a single element antenna of equal length. A planar line monopole antenna element is the most suitable choice for MIMO antenna system. The tool which we have used to design the antenna was HFSS. The designed antenna has been fabricated on the FR4 substrate. Network analyser has been used to test the fabricated design. MLA antennas for RFID based on multi objective optimization. The purpose of this design is to made effective meander line antenna for RFID purpose. The multi-objective system is faster to converge than the single goal one. However, considering that SWRs of 1 and 40 at pattern frequencies can be considered Pareto most useful for the former method, the solution of the worst-case components may be appeared more meaningful, that is, an excellent decision rule, even though it is either ruled or protected in the optimal Pareto set. In our case, for the purpose of reducing the size of transponder, a meander-line antenna (MLA) is an attractive choice. This class of antennas provides the largest size reduction at a given frequency at the expense of a narrow bandwidth. Compared with the PIFA antenna, there is an advantage that the MLA is relatively easy to catch larger relative bandwidth. A meander-line antenna can be realized by bending the conventional linear monopole antenna to decrease the size of antenna. The influence of the meander part of the antenna is similar to a load and the meander line sections are considered as shorted-terminated transmission lines. The meander line section can be modeled as an equivalent inductor. In the far-field pattern, in the result of the cancellation of magnetical fields, the transmission lines of a meander line antenna do not radiate fields. The radiation fields will be radiated from the vertical pars of MLA. It is a smaller area, but the radiation resistance, efficiency and bandwidth decease. In order to find the best antenna solution, different values of meander width are simulated and studied.

Modal study of proposed electrically small antenna

The proposed antenna consists of a microstrip-feed-line of length L_f and width W_f on the top surface of the substrate and a meander-line connected to the ground plane on the bottom of the substrate. First, the modal analysis of the microstrip-feedline and meander structure has been studied, separately. Then the modal analysis of the entire

structure of the antenna has been studied. The commercial software package HFSS [11] has been used for the modal study.

1. In Modal analysis of the microstrip-feed-line the first two characteristic angles of the microstrip-line. It can be seen that the characteristic angle of the first two modes are near 270□ and store electric energy. Thus, none of the modes of the microstrip-line are within the range of 1 to 4 GHz resonant.
2. Modal analysis of the meander structure: Fig1 shows the first two characteristic angles of the meanderline attached to the ground plane. It can be observed that only the first mode is resonant and its characteristic angle crosses 180□ at the frequency of 2.91 GHz.

3) Modal analysis of the proposed antenna: Characteristic angles of the entire antenna structure are shown in Fig.2. It can be seen that the first mode resonates at the frequency of 2.52 GHz since its eigenangle crosses 180□. Fig. 3 shows the first eigencurrent of the proposed antenna. The first eigencurrents on the meander structure in this stage and the previous stage have the same profile and flows from one side to the end of meander-line. But in the microstrip-line associated with the meander structure, the flow path of the first characteristic current is longer than the alone microstrip-line, and it is not a straight line. When this parasitic structure is located in very close ($\lambda_0/85$) to the microstrip-feed-line, extending theflow path increases bandwidth. Due to the coupling between the meander structure and microstrip-feedline, the resonant frequency has been shifted about 390 MHz [12]. In the simulation, the proposed antenna is analyzed with a finite substrate and volume equivalence principle (VEP).

Design and implementation

For designing the proposed electrically small antenna, five steps are considered. In step 1, the antenna shape includes a microstrip-feed-line on the top surface of the substrate and a conventional ground plane on the bottom of the substrate. In step 2, a square slot is created on the ground plane. In step 3, a straight line is connected to the ground plane. In step 4, two gaps of length L1 are created on the square ring. Finally, the straight line is replaced by a meander-line. In [13] and [14], due to the presence of the microstrip-feed-line and the meander-line on the top surface of the substrate, the overall size of the antenna has become larger. In step 5, it can be seen that the meander-line acts as the principle radiation component of the antenna structure because there are strong currents on the meander-line.

Parametric study

To study the results of various parameters on the overall performance of the proposed antenna, a parametric study has been performed. The antenna has been simulated through using High Frequency Simulated Software (HFSS). In the proposed antenna, the meander structure is located in very close proximity to the microstrip-feed-line, approximately $\lambda_0/85$, and it provides a large inductance to achieve the desired impedance matching. The microstrip-feed-line width influences the imaginary part of the impedance. Increasing the length of M_1 or decreasing M_2 of the meander-line as shown, provides a larger inductance. Fig. 5 shows the reflection coefficient and gain of the proposed antenna for distinct values of the meander length (M_1), meander width (M_2), space between two strips (M_3), gaps length (L_1), feed length (L_f) and feed width (W_f) From Fig.5(a), it can be seen by increasing M1, the resonant frequency is decreased. Moreover, the increase in M2 or the decrease in M3 increases the resonant frequency as shown in Fig. 5(b) and (c). In general, by reducing the coupling between the microstrip-feed-line and meander structure, the resonance behavior shifts towards lower frequencies. From Fig. 5(d), it can be seen by increasing L1, resonant frequency is increased. As can be seen in Fig. 5(e) and (f), the length and width of the feed-line only cause the frequency shift. As can be seen in Fig. 12, varying the parameters causes a slight change in the gain curve. However, due to the resonant frequency shift, there is little change in the gain value.

RESULTS AND DISCUSSION

To validate the design process of the proposed electrically small antenna, it has been fabricated on a Rogers RO4003 substrate with height = 1.524 mm, ε_r = 3.55 and tan δ = 0.0027. In this design, by considering that the ka value for electrically small antenna must be smaller than 0.5, the whole size of the proposed antenna is 8.5 mm × 8.5 mm that at 2.4 GHz frequency ka = 0.302. A circuit simulation result has been also obtained using ADS software. The measured results show that a -10dB impedance bandwidth from 2.28 to 2.5 GHz is achieved. It can be observed that there is a frequency shift about 120 MHz (2.52 GHz to 2.4 GHz) between two full wave simulation, i.e. HFSS, and the modal analysis, i.e. HFSS, results. This difference is due to the excitation method, different numerical methods, i.e. MoM and FEM, and loss tangent of the substrate. In the modal analysis, the loss tangent of the substrate is neglected; however, the difference between lossless and lossy substrate is small [16].

CONCLUSION

An electrically small antenna is proposed at 2.4 GHz frequency using characteristic mode theory and metamaterial-inspired antenna. The antenna consists of a microstrip-feed-line on top of the substrate and a single parasitic material unit-cell on the bottom of the substrate. This antenna has a small dimension of 8.5 × 8.5 × 1.524 mm^3 (0.068 λ0 × 0.068 λ0) and ka value of 0.302. The antenna performance is studied numerically. This antenna is one of the smallest electrically small antennas available at this frequency. It can be a good for future compact wireless devices that require a compact and simple antenna structure with a good performance.

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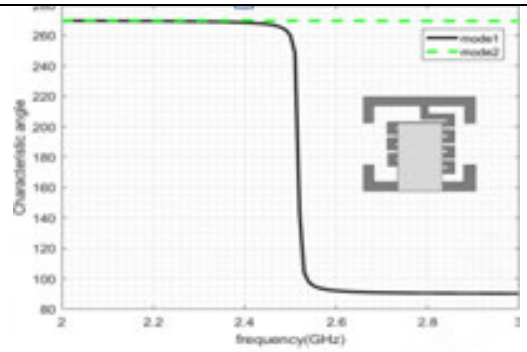

Fig 1:Characteristic angles of proposed antenna

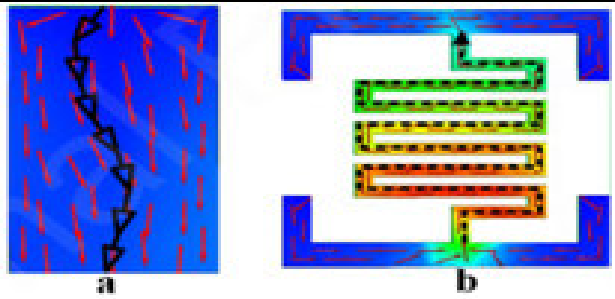

Fig. 2 The first eigencurrent of the proposed antenna a.Microstrip line b.Meander structure

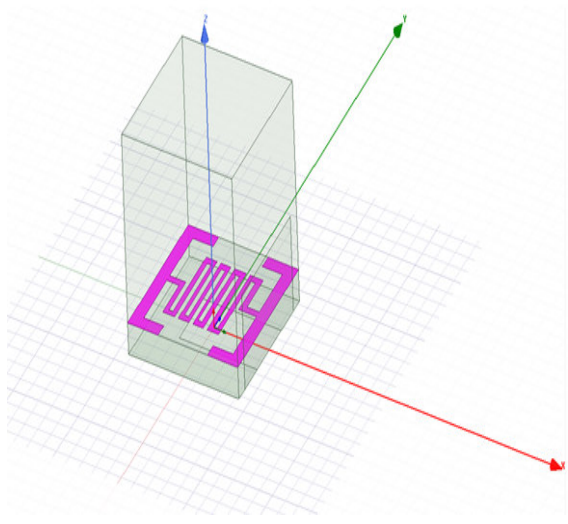

Fig3: Meander line antenna design using HFSS

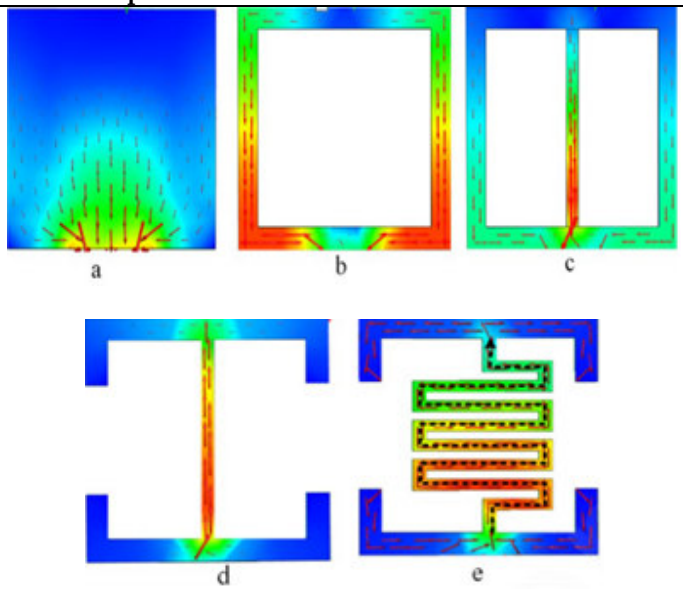

Fig 4. Step 1-5 of the proposed antenna

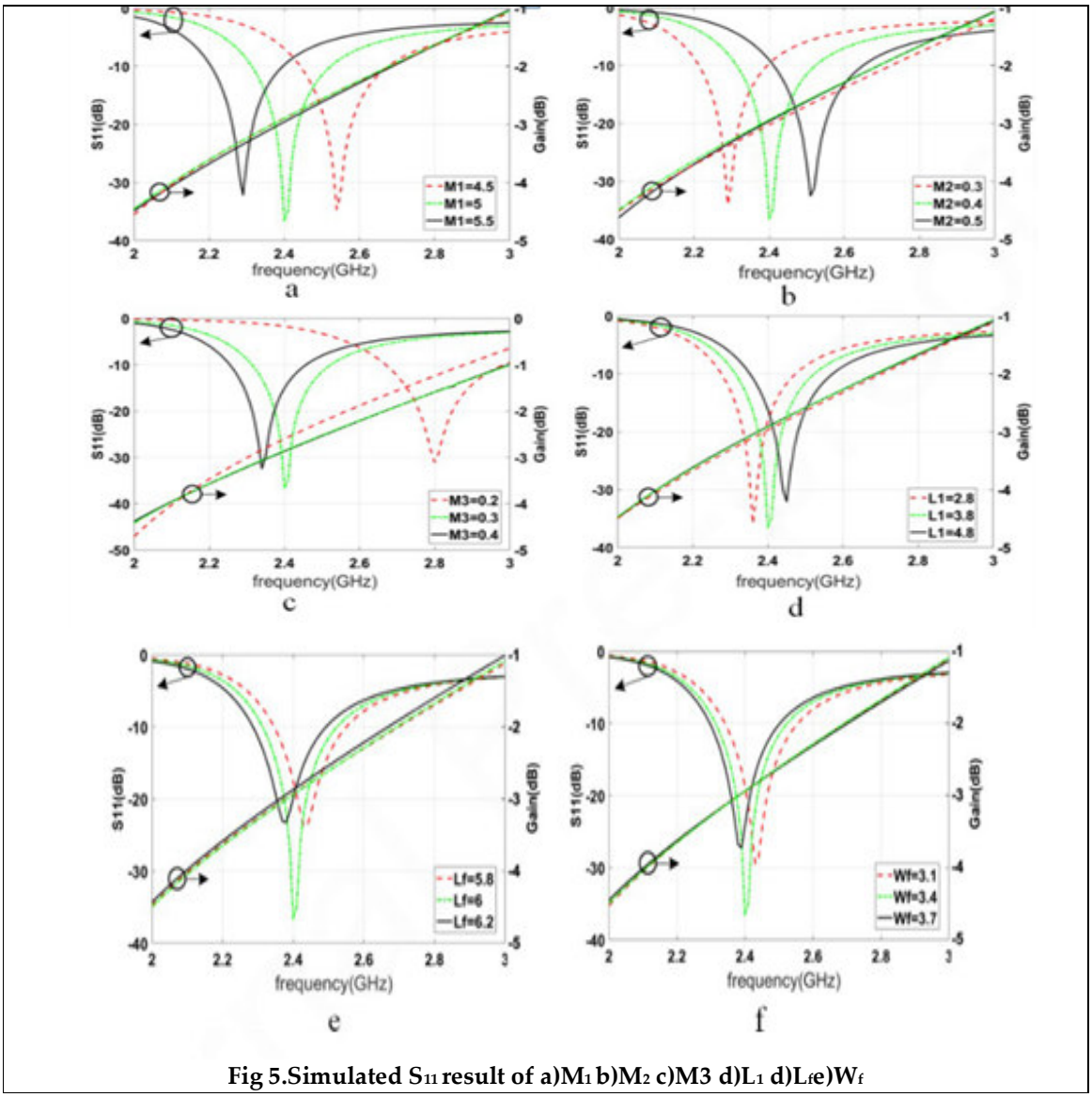

Fig 5.Simulated S_{11} result of a)M_1 b)M_2 c)M3 d)L_1 d)L_fe)W_f

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RESEARCH ARTICLE

Heavy Metal Accumulation by Plants as a Result of Diwali Fire Craker Emission in Urban Areas of Bhubaneswar, Odisha, India

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ABSTRACT

Diwali has been one of the largest festivals in Hindu religion which usually fall in the month of October to November every year. At the time of the festival days excessive amount of burning of fire crackers takes place mostly in evening time. Fire crackers pollute the environment with noise, particular matters and chemicals. There are some reports which is known the impact of particles of fire crackers but none of them are plants. The present study is performed to know the impact of fire crackers on plants and environment. The plants parts which are collected after Diwali in the year of 2019 at 6 different areas in Odisha, India. After the experiment the most amount of chemical which is used in fire crackers is CaO (Calcium Oxide), which is a white, caustic, alkaline, crystalline solid. The fire crackers shows more impact on plants. The study shows that plants are also susceptible to the chemicals emitted by the fire crackers when they are burn out.

Keywords : Diwali, Festival, Plants, Crackers, Strontium

INTRODUCTION

Diwali is commonly known as the festival of lights. It is mostly celebrated, so the fire crackers are burnt by the people. Diwali festival usually occurs in October / early of November and this is celebrated so vastly (1). Usually people startburning fire crackers before 2- 3 days. Fire crackers are exploding in the atmosphere and shows the impacts on plant. After the experiment it is found that in plants after the Diwali the chemicals contain are SiO_2, P_2O, SO_3, Cl, K_2O, CaO, TiO_2, MnO, Fe_2O_3, NiO, CuO, Zno, Br, Rb_2O, SrO and so on. In the recent time the air quality impacts on plants is too dangerous which on shows badly. To this respect special air quality degradation on plant

that has been reported due to bursting of fire crackers in Diwali (2). The chemicals and their components that are used in the crackers are Strontium, Calcium, Sodium, Barium, Copper, Magnesium, Aluminium, Titanium etc. Due to burn of huge amount of fire crackers mainly on the day of the festival and the day before and after the festival (considered as Pre-Diwali and Post- Diwali days) (3). The gases which has been out of the burnt fire crackers are in such a manner it is trashed that the gases are fixed with the plant that are to be detected by the experiment. Fire crackers affects the environment, some of the rockets set fire to huts, heaps of dry grasses and houses. In the present study, we found many chemicals but CaO is found much amount in the plant species. The CaO isused as the burning particle in the crackers.

METHODOLOGY

COLLECTION

The plants and plants parts has been collected from different 6 areas of Odisha. The places where the plants have been collected are Lakmi Sagar, Jharpada, Samantarapur, BDO Colony, Palla, Sagwanbagicha. We had choose those places because there was more amount of burst of fire crackers as compared to other places.

IDENTIFICATION

The plants which we have collected we identified those plants and named it. Then we have send those plants to the ATC Laboratory. Then it has been examined and identified that how much amount of fire crackers are found in the plants.

RESULT AND DISCUSSION

Study on the documentation of plants which shows impacts on Diwali crackers in different areas of were carried out after the Diwali. The data on the impact of Diwali fire crackers was collected through interaction through the specialist (4). In Hindu custom it has been accepted that Diwali has been one of the largest festivals in Hindu religion which usually fall in the month of October to November every year. The six plant samples were collected from six different areas of Bhubaneswar, Odisha i.e Kaniara (*Cascabela thevetia),* Arakha (*Calcotropis ginantea),* Mandara (*Hibiscus rosa-sinansia),* Malati (*Aganosma heynei),* Kaicha kakudi (*Coccinia cordigolia),* Tagara (*Tabernaemontana divaricate).* Burning of sulfur nitrates, magnesium, aluminum, paper, and different materials contained in firecrackers produces air contamination during Dials. During XRF analysis the elements like CaO, SO_3, ZnO, NiO were found to be highest in plant parts after Diwali (Table 1). This study showed that the burning of crackers on Diwali is a solid wellspring of air contamination which contributes an altogether high measure of metals in air.

CONCLUSION

The study based on effects and impacts of crackers used in Diwali on plants and plants parts. The present study helps to realise that Diwali which is the festival of lights, but we, the humans have made it into a noise and pollution. Not just human beings, but also animals and plants are impacted by the fire cracker culture. If plants could speak, they would definitely beg cracker lovers not to use crackers during Diwali. After crackers burst in the air, they emit toxic gases in the atmosphere that are extremely damaging to the health of all living beings, including plants. This study greatly revels that the plants are living and they need cares during lighting crackers and fireworks. Plants feel suffocated and cry for help when Diwali crackers burst.

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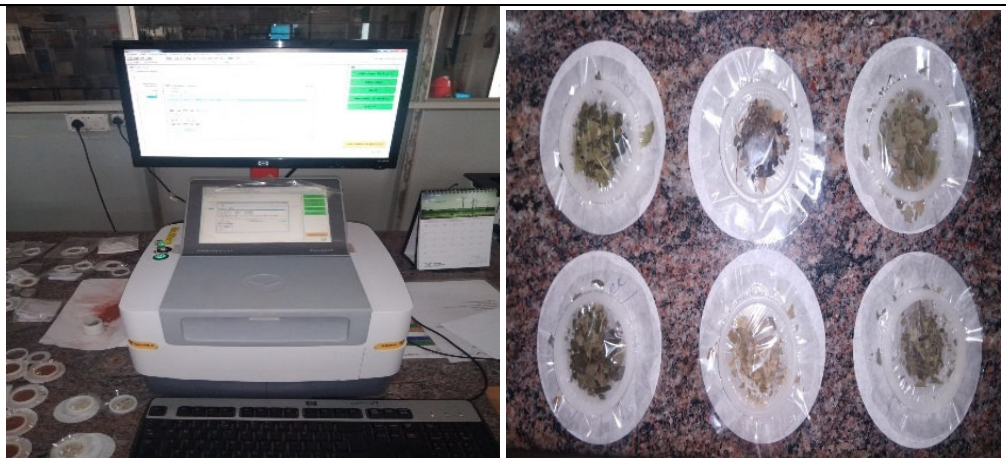
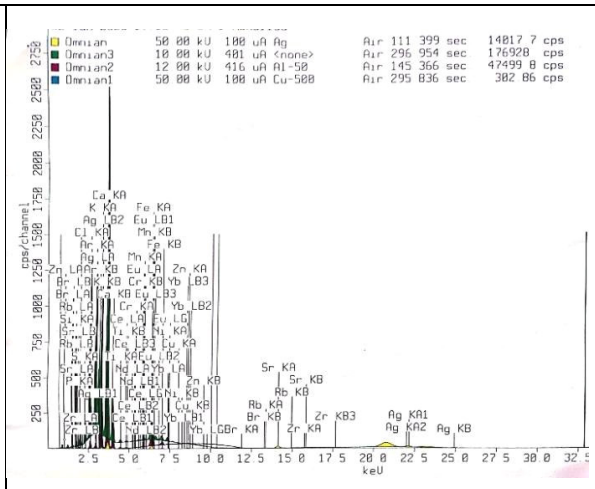
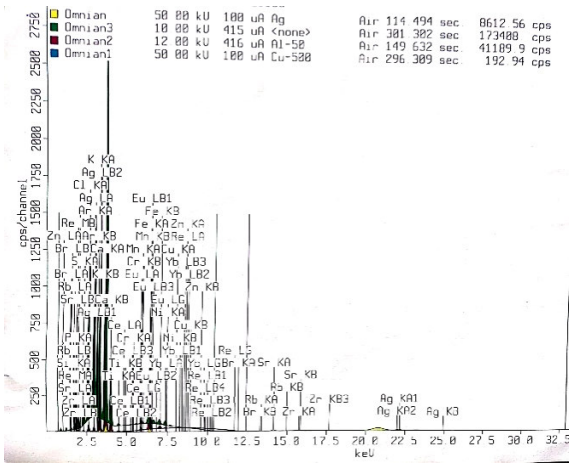
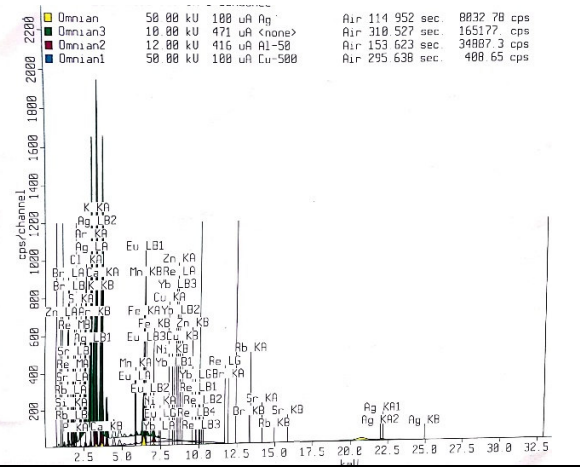
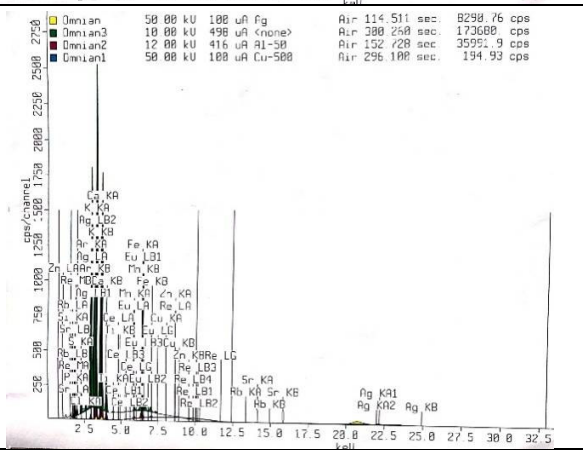
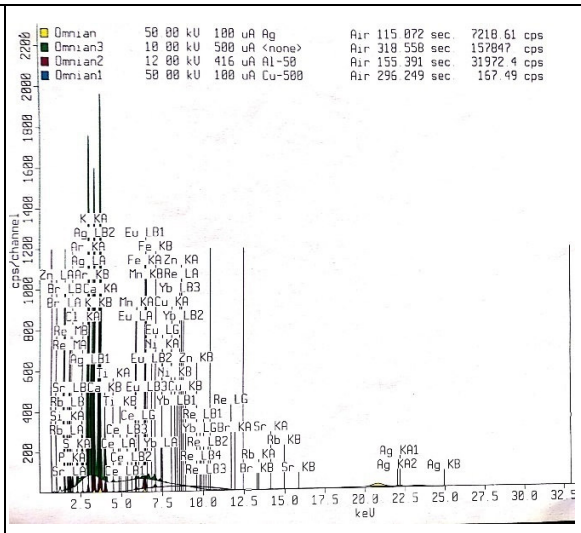
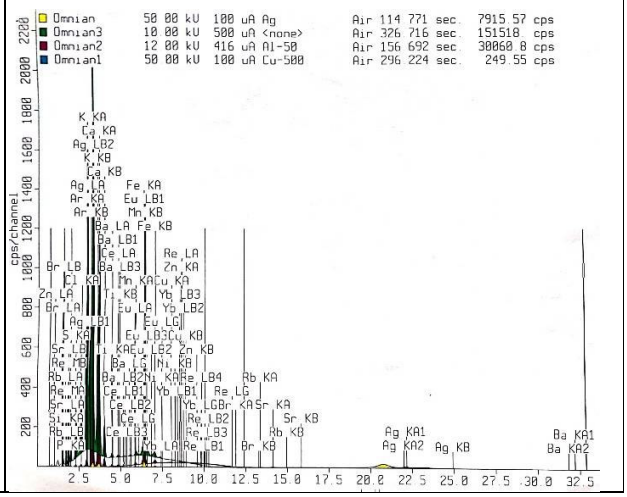


Fig 1. During experiment (data analysis by XRF)

Table 1. Elemental analysis by XRF method

Sample collected area: Lakhmi Sagar	**Common name:** Kaniara **Botanical name:** *Cascabela thevetia* **Elements detected:** SiO_2, P_2O_5, SO_3,Cl, K_2O,CaO, TiO_2, Cr_2O_3, MnO, Fe_2O_3, NiO, CuO, ZnO, Rr, Rb_2O, SrO, ZnO_2, CeO_2, Nd_2O_3, Eu_2O_3, Yb_2O_3, CO_2	

Jharpada	**Common name:** Arakha **Botanical name:** *Calcotropis ginantea* **Elements detected:** SiO_2, P_2O_5, SO_3,Cl, K_2O,CaO, TiO_2, Cr_2O_3, MnO, Fe_2O_3, NiO, CuO, ZnO, Rr, Rb_2O, SrO, ZrO_2, CeO_2, Eu_2O_3, Yb_2O_3, CO_2, Re	
Samantarapur	**Common name:** Mandara **Botanical name:** *Hibiscus rosa-sinansia* **Elements detected:** SiO_2, P_2O_5, SO_3, Cl, K_2O, CaO, TiO_2, Cr_2O_3, MnO, Fe_2O_3, NiO, CuO, ZnO, Br, Rb_2O, SrO, Eu_2O_3, Yb_2O_3, CO_2, Re	
BDO Colony	Common name- Malati **Botanical name:** *Aganosma heynei* **Elements detected:** SiO_2, P_2O_5, SO_3, Cl, K_2O, CaO, TiO_2, Cr_2O_3, MnO, Fe_2O_3, NiO, CuO, ZnO, Rr, Rb_2O, SrO, ZnO_2, CeO_2, Eu_2O_3, CO_2, Re	

Palla	**Common name:** Kaicha kakudi **Botanical name:** *Coccinia cordigolia* **Elements detected:** SiO_2, P_2O_5, SO_3, Cl, K_2O, CaO, TiO_2, Cr_2O_3, MnO, Fe_2O_3, NiO, CuO, ZnO, Rr, Rb_2O, SrO, CeO_2, Eu_2O_3, Yb_2O_3, CO_2, Re	
Saguanbagicha	**Common name**: Tagara **Botanical name**: *Tabernaemontana divaricate* **Elements detected:** SiO_2, P_2O_5, SO_3, Cl, K_2O, CaO, TiO_2, Cr_2O_3, MnO, Fe_2O_3, NiO, CuO, ZnO, Br, Rb_2O, SrO, BaO, CeO_2, Eu_2O_3, Yb_2O_3, CO_2,Re	

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RESEARCH ARTICLE

Analog Electronics Circuit Simulation in Dymola

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ABSTRACT

For dynamic behaviour modelling and simulation and the interaction between systems of many fields of engineering, such as mechanical, electrical, thermodynamic, hydraulic, pneumatic, thermal and control systems, Dymola is offering new and revolutionary solutions.Three separate efforts have been made in three different institutions in recent years to provide electronic circuit modelling and simulation capability as an object-oriented general-purpose environment for the design of physical structures in Modelica.There is no hard-coding domain knowledge to use in Modelica software.Not physics, but only mathematics, understands Modelica.Accordingly, all subject information shall be included in the layout.Recent software and symbolic algorithms have enabled the complete electronic circuit simulator to be implemented in Modelica without sacrificing the runtime for the resulting simulation.In this process, the improvement of the transparency and ease with which the code is maintained is significantly improved, and the flexibility to combine the electronic models with the mechanical and thermal ones dramatically improves. Analog inverter circuit using BJT, comparator , and noninverting amplifier using OPAMP were designed in Modelica modeling of Dymola software and simulation results were obtained.

Keywords: Electronic circuit simulation, modeling, Modelica, simulation, analog

INTRODUCTION

Dymola was designed to be an equations-based declarative rather than a proceedings-based language.The causality of each equation is determined automatically by the model compiler, i.e. the variable the equation needs to solve..A compiler is invoked to convert implicit (declarational) model specifications into an express (procedural) state-space shape in symbolic formula manipulation algorithms.An off-shelf CSSL-type simulator can then simulate the resulting simulation code.The semantic gap between the original implicit model specification and the outcomes may be quite large from a historical point of view.However, from a use perspective, OOMLs are a real revolution, as they allow modellers to treat all models in the same way.The modelling environment for control systems no longer needs to be distinguished from one for electronic circuits.Although it is possible to build an OOML model of a circuit by

using conventional Spice implementations to be a little slower than the corresponding compilation, the results of simulation coding in the exercise speed can be equally efficient.In the meantime Model [1] has substituting the most commonly used OOML for Dymola[2].While Elmqvist developed and commercialised the Dymola language as a proprietary code, Modelica was created and not owned by a standard committee.Anyone can develop a compiler and a basic simulation engine based on the language of the Modelica and, indeed, several Modelica implementations already exist.Modern Dymola[3] is an environment based on Model Language Specification among several M&S environments.Dymola offers a visualisation and animation of simulation results, the Modelica compiler, a CSSL-type simulation engine, and several other tools for model manipulation including linearization engines. Dymola also has the graphical user interface (GUI).This M&S environment is Dynasim 's commercial code.Open Modelica [4] is a free (open source) Modelica compiler implementation.Open Modelica [4] is a free (open source) Modelica compiler implementation.A CSSL-simulation engine is provided for the code.It also offers a (simple) results visualisation programme, but for the visualisation of their simulation results, many open modes users choose Matlab[5].As a GUI to OpenModelica, MathModelica Lite [6] can be used.The advantages and disadvantages for Dymola as well as OpenModelica.Because the code is more developed, easier to use, has more features, is more professional, and creates more functional, simulation code, industrial users can prefer Dymola.Academics may prefer OpenModelica, as the code is free and open-source, allowing additional resources to be developed and other algorithms to be put in place easier than Dymola [7].This article is based on Dymola as it focuses on the conception of Modelica libraries, not on new algorithms.

Analog electronic circuits simulation in Modelica

There are three modelica libraries of analog electronic circuits are available (a) The modelica standard library (b) SPICELib (c) BondLib. The analog inverter circuit using BJT, Comparator circuit, and noninverting amplifier circuit using OPAMP are designed and simulated in Modelica.The individual inputs and output waveforms are shown as simulation result.

Modelica denotes a language definition as well as a model library in Modelica language.The Modelica library is called the standard library of the Modelica, which is in the Public Domain and is intended for all Modelica implementations.A sub-library of models containing electronic circuit components, one for digital (logic) circuit elements and another for analog circuit components, contains a Modelica standard library.The analog electrical library contains model elements of the passive electrical components as well as the transistor and diode models and the current and voltage models (resistors, condensers and inductors).The standard library transistor models are significantly simpler than those in Spice 's applications.The standard library transistor models are significantly simpler than those in Spice 's applications.These models are therefore not suitable for integrated analogue circuit design.Spice implementations also offer different types of analysis, especially DC analyses, AC analyses and temporary analyses.For transient analysis only, Dymola is designed.The ease of transistor models in the standard library, on the other hand, is also beautiful.These models can be very effectively simulated and the large transistor circuits can be simulated efficiently.In addition, teacher who wish to teach students the basics of analogue circuit design can be rewarded for the simplicity of these models.Finally, the standard library also offers models of thermal analog circuit components which permit circuit designers to model, and simulate electronic circuit thermal storage and dissipation not possible in Spice, as electrical circuit models are simulated alongside mechanical system models, allowing Dymola to model and simulate mechatronic systems in an elegant mannerand simulate mechatronic systems.The modelling and simulation of electronic circuitry using the Modelica Standard Library may be illustrated using a simple analoginverter circuit.The BJT circuit diagram of the analogue inverter is illustrated in figure 1.Essentially, the circuit diagram is identical to the circuit diagram corresponding to the preprocessor Spice by any schematic capture programme.A single bipolar crossover transistor (BJT) is provided in the circuit.In the modelica language itself, Modelica "Soft," contrary to Spice's "hard" encoding its device models in Fortran or C, encodes the entire field knowledge of its models.The compiler Modelica encapsulates only math.As a result, Modelica models are significantly easier than Spice models to understand, maintain and upgrade.In Dymola, four individual entities represent each object (model).This consists of an iconic (graphic) image used to graph the model to be invoked

hierarchically at a higher level; a diagram (graphic) representing the inner structure of the template using the interconnected set of submodels; a representation equation (textual) that permits the model to be described with (implicitly formulated) equations;In the example above, the diagram layer describes the inverter circuit.The Modelica compiler can convert the inverter circuit model into a state-space model.The Dymola simulator uses the numerical ODE solver DASSL by default.For the complete simulation, it took 0.04 sec.The circuit undergoes a transitory period during the initial period as the model did not start in a recessed state.In Spice, the user would normally precede the transient analysis by calculating a DC OP point that would eliminate the transition from the results of the simulation.

SPICELib

A few Modelica users have written their own library in addition to the Modelica standard library.Some of these libraries are business libraries, while other libraries are free.One such free library is SPICELib. PSpice is one of Spice's most common dialects.Many models are therefore familiar with PSpice equipment parameters and PSpice parameter sets for most commercially available electronic devices have been identified.SPICELib has a long tradition of offering different models for the different types of analysis. For example, one SPICELib model contains several models, one for DC analysis and another for AC analysis and one for transient analysis. SPECILIB follows the traditional Spice philosophy.As a result, the SPICELib connectors are incompatible with the electrical library's standard connecting systems and, therefore, unfortunately SPICELib and the standard component models cannot be mixed.Just as with the standard library, the SPICELib component models using the equation layer have been implemented.These models are, however, much more complex now, and are less understandable and easier to maintain.At the top, these are full flavours for circuit design that can be used.Moreover, it is particularly convenient for experienced PSpeice users to switch to Modelica if they decide on PSPice and SpICELib similarity and the availability of separate models to the various analysis types.Our demo circuit cannot however be simulated in SPICELib at present because SPICELib offers only MOSFET models.There have been no releases of the BJT and JFET models.

BondLib

The BondLib library is another free, bond-graphy library.Domain-independent modelling is provided in Bond graphs.Bond graphs are the most fundamental paradigm of still fully object-based graphic modelling.The need for modelling using the equation layer can be greatly reduced by mapping higher-level models to a link graph layer, which enhances the understanding and maintenance of the models. BondLib has an electrical analog subsection, which appears to be quite similar to the respective subsection of the Modelica Standard Library.However, each component model is decomposed to a bond graph layer graphically more closely.BondLib also includes real Spice models, in contrast to the standard library.However, its Spice models are based on HSpice ([14]), another Spice dialect with sets of device parameters that differ slightly from PSpice.HSpice and BondLib provide their device models with diverse levels of complexity.More complicated models at higher level have more device parameters and are therefore slower to implement.BondLib contains only temporary analysis models, just like the standard library.For this reason, the BondLib power connectors are compatible with the standard library electrical connectors, and both models can be mixed freely.In BondLib, however, the BJT models contain a (green) additional port which denotes the substratum, and all device models have an additional (red) thermal port.The BJT model consists of an internal model BJT plus the collectors, emitters and (nonlinear) resistors, a base-substrate interconnection diode and a nonlinear straying capacitance between the external foundation and the internal collector nodes. (in the case of laterally diffused BJT).It includes the typical nonlinear gummel-poon crossing ability, the true diode characteristic, and a stray conductance (with numerical motivation).The bond graphic device models are at the next lower (still graphic) level.Small equation models implementing the primitive graphs are below that level.At first there are 2624 unknown equations in the model.Most of these equations are trivial equations, however, which are removed compilation in the process.There are three state variables and 162 algebraic variables in the simulation model.It is as straightforward as a complex model can be expected.Each of the three diodes has a one-state crossover capacitance.External stray capacity is a dependent capacity that does not result in a supplementary state variable.It is removed by a symbolic index reduction during the compilation process.There are no more than two state variables in

the standard BJT model because it does not include a substrate model.The BondLib model compilation is obviously slower than the standard model, but Dymola is very effective in building it.Both builds only consume one-second splits.The simulation is also slower than the equivalent circuit using the standard library, as the model is significantly more complicated.The slow-down of the simulation is however less than an acceptable factor of 2.First of all, BondLib's BJT model has the basic, collector and emitter connexion resistors (in accordance with the Spice philosophy) whereas the standard library's BJT model doesn't.These are externally to be added.It should not neglect their influence.In particular, the basic resistor (about 1000 ohm) is quite large.Secondly, BondLib supports DC analysis that is not contained in the standard library.A newton iteration traditionally calculates a DC OP point in Spice.That is not done by BondLib, but rather by increasing the source, it computes a DC OP point.If all the active devices are switched off initially and all sources initially at zero, then all the voltages and currents are zero physically plausible.We can therefore begin with this solution, ramp all sources up to their initial values, and keep them for a while before the transient analysis begins.BondLib provides the source of the ramping to enable the user to specify the time for each.

AC analysis inBondLib

We need an input / output model to linearize around a suitable stable point.A good stationary point is the final state of temporary simulation.It is automatically saved by Dymola in the dsfinal.txt file.We must return quickly to the modelling window, select the Operating Verstorage Circuit model and return to the simulation window.We must now read as initial states the final values of the transitional analysis.The Continuance / ImportInitial... command in the simulation pull-down menu requests you to select the readable file, the dsfinal.txt file.Then the circuit around the initial state must be linearised.This is also done by the Linearize command in the simulation pull-down menu.The linearized model is stored in the dslin.mat file.The actual AC analysis is not conducted in Dymola.itself, but instead using Matlab's toolbox control systems.The bandwidth of the operating amplifier is approximately 1 MHz.The amplitude and phase features are both beautifully flat up to this frequency.BondLib is not specific to the approach described here.The same approach could just as easily have been applied to model the high gain operating amplifier circuit using the standard library.The approach, however, is unique to Dymola M&S.Nothing supports linearization in the specification of the modelica language.Therefore, other Modelica implementations either will not support this feature or at least will not support it the same way.The suggested approach is more object-driven than SPICELib 's approach, because all three types of analysis can be carried out using the same model.The maintenance of the code is simplified.However, SPICELib 's approach is easier to use, since it allows modellers to analyse the AC using one single command, as in Spice.Using OOMLs to model and simulate electronic circuits offers several striking advantages over using Spice.These are listed now.

Mechatronics

Industry now constantly requires computer and mechanical circuit co-simulation.For instance, automobiles manufacturers want the electronic control circuit of their engines simulated with the engines.It even got its own name, mechatronics, the area was so popular.In Spice it is not possible to simulate mechatronic systems because Spice allows modelling systems other than analogue electronic circuits.Mechatronic structures of OOML like Modelica.

Thermalanalysis

Heat dissipation is a big concernwith the increasingly rising density and speed of electronically integrated circuits.While Spice allows the simulation of an electronic circuit at different temperature values, it does not feature.Using an OOML and especially one based on bond graph technology, performing electronic circuit thermal analysis is a breeze.

Softwareupgrades

The built-in DC analysis often do not converge on their analogue circuit to produce an automated ramping characteristic.Similar demands can be processed in a few hours using a language such as Modelica because Modelica stores its specific domain knowledge in the model instead of in the compiler.

Teaching

Although spices can be used to check circuits, they cannot easily be used to demonstrate how transistor models operate.The reason is that Spice transistor models are black box models that can only be viewed from outside.Although many of the Spice handbooks display equivalent replacement circuits based on the transistor models, the student does not have access to their internal signals.The student can actually view the replacement circuits and dig them to any level he or she chooses, especially when embracing the approach adopted by BondLib, even down to the bond graph models at the bottom of the graphic model here.This allows BondLib to be used in the teaching of basic semiconductor technology effectively and efficaciously.

CONCLUSION

Modelica has been an outstanding tool for scientists and engineers to share information on complex systems.Models can be freely interchanged and combined to simulate mixed energy systems.It consists of sub-libraries for electrical , mechanical and hot systems, a block diagram library describing control structures, a state graph library describing discrete structures, a network library for convective flow modelling systems, and a widely used scientific library and a physical library for universals constants.. The standard library is easily the largest volume of information about dynamic systems freely available on the public domain.It is planned to become the most important one-place-shop-all tool for physical system modellers worldwide.There are also growing numbers of free libraries available on the Modelica website, including SPICELib and BondLib, maintained outside the standard library.These libraries should undergo frequent modifications and enhancements.Until now, we have focused primarily on analog circuits. Analog inverter circuit using BJT, Comparator and noninverting amplifier circuit using OPAMP were designed and similuated.

There is also a definite need to simulate mixed analog and digital circuits, such as switched power converter circuits, that neither Spice nor LogicWorks can handle.

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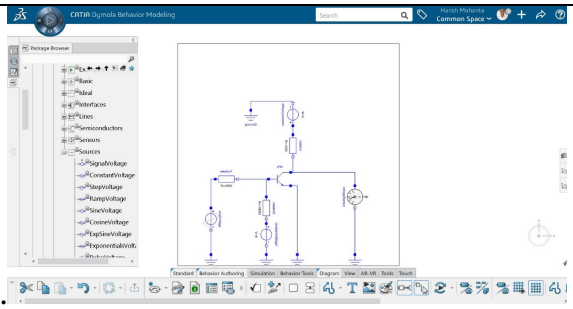

Figure 1. Analog inverter circuit using BJT

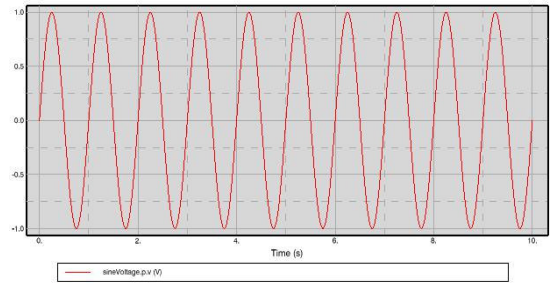

Figure 2. Input signal at BJT inverter circuit

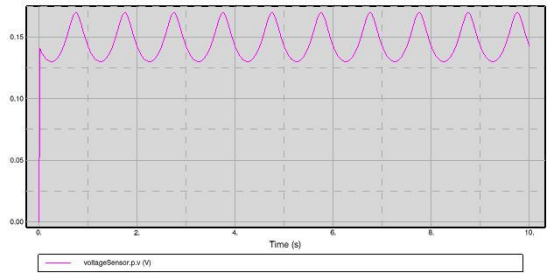

Figure 3. Output signal of BJT inverter circuit when input is sinusoidal signal

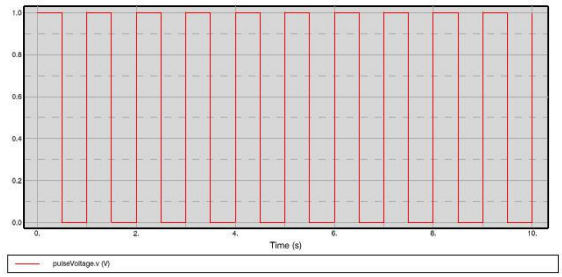

Figure 4. Periodic pulse input to the BJT inverter circuit

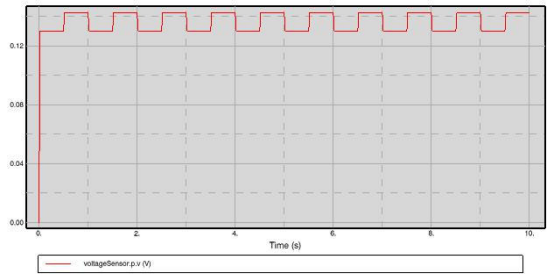

Figure 5. Output of BJT inverter circuit when input is periodic pulse signal

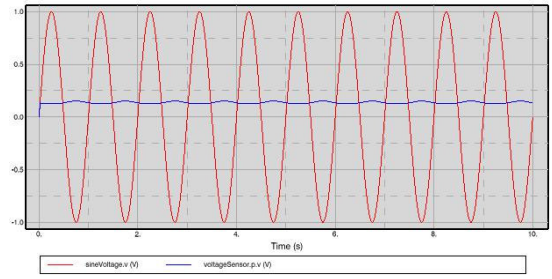

Figure 6. Both input and output wave form

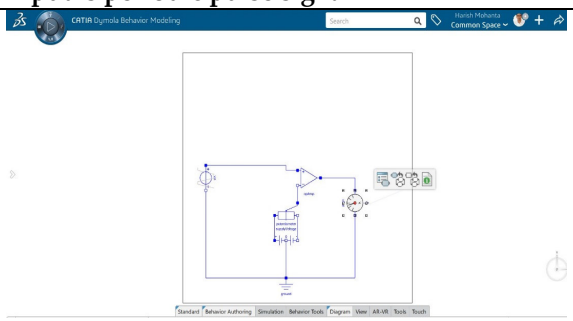

Figure 7. Comparator circuit design

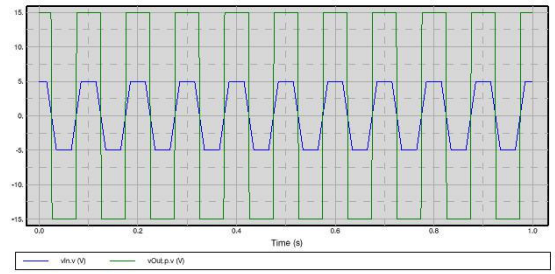

Figure 8. Input and output waveform of comparator circuit

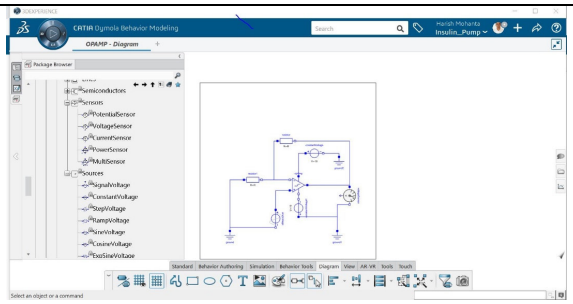

Figure 9. Noninverting amplifier using OPAMP

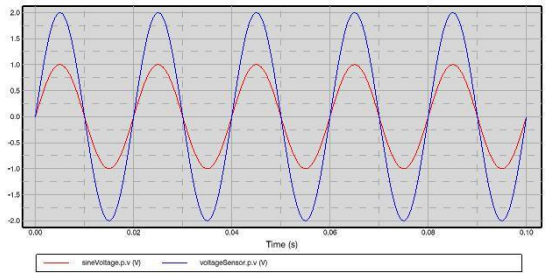

Figure 10. Input and output waveform of noninverting amplifier

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RESEARCH ARTICLE

Preparation and Testing of Dual Blended Biodiesel of Castor and Mahua in VCR Diesel Engine

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ABSTRACT

Alternative fuel forinternal combustion engine is a topic which is attracting many researchers in recent times due to depletion of fossil fuels. It also reduces pollution and protects against global warming. Among different alternative fuels, biodiesel is regarded as a major source as a substitution fuel for internal combustion engine which has similar properties with diesel. India has a great scope for the production of biodiesel from nonedible oil seeds due to abundance of vegetable plants. Raw vegetable oils can be used directly or blended with diesel to run diesel engines. However the engine modification is a challenge for its usability aspect. Also there may be occurrence of serious problems in fuel ignition if the viscosity of the oil is not taken care of. In the present work, a dual blended biodiesel of Castor and Mahua is used as fuel for variable compression ratio diesel engine to test its performance without any modification of the engine. The performance results obtained are within acceptable limits.

Keywords: Performance, Biodiesel,Blend, Castor, Mahua

INTRODUCTION

Biodiesel is accepting extraordinary consideration as a result of its fuel properties and similarity .It has preferable properties over that of petroleum diesel.It is a naturally agreeable fuel that can be utilized in any diesel engine. Biodiesel is an elective type of diesel got from either plants and plant item or creature fat [1]. It is an elective diesel fuel, which is supplied by synthesizing vegetable oil or creature fat with liquor, such as methanol or ethanol, for example.That synthetic response which changes over a vegetable oil or creature fat to biodiesel is classified "transesterification" [2]. The synthetic response used to make biodiesel requires an impetus. An impetus is typically a substance, which added to the response blend to accelerate the response.

Since biodiesel is made altogether from consumable and nonedible oils, it doesn't contain any sulphur, sweet-smelling hydrocarbon, metals or unrefined petroleum deposits. The lacking of sulfur implies a decrease in the development of corrosive downpour by sulfate emanations which create sulphuric corrosive in our air. The diminished sulphur in the mix will likewise diminish the degrees of destructive sulphuric corrosive assembling in the motor crankcase oil after some time [3].

Ghaly et al. [4] revealed that the exploration on the creation of biodiesel has expanded surprisingly lately as a result of the requirement for an elective fuel which invests with biodegradability , low harmfulness and sustainability.Deepanraj et al. [5] portrayed that the less mixes of biodiesel expanded the brake warm effectiveness and limited the fuel utilization. Moreover, biodiesel mixes produce lower motor emanation than diesel.

Biodiesel is delivered by means of the transesterification response among oils within the sight of a suitable impetus [6]. All in all, either homogeneous or heterogeneous, and salt or acidic impetuses can be utilized in the transesterification response to boost transesterisation response execution and upgrade biodiesel creation returns [7]. Transesterification process within the sight of salt impetuses is a general procedure for biodiesel creation, since this response within the sight of soluble base impetuses is around 4,000 overlap quicker than within the sight of acidic impetuses, making the procedure all the more monetarily feasible [8].

In the present work, equal amounts of castor oil and mahua oil are mixed together for better outcome. And furthermore it is another method of making biodiesel by including or mixing of these two oils combine. When biodiesel is at first mixed, as it ventures to every part of the conveyance arrange until it arrives at the end goal of the fuel siphon or capacity tank. Biodiesel can be mixed with other fuel to deliver mixed biodiesel fuel base on weight premise or volume premise. The last result of blending ought to be homogeneous. Diesel fuel and biodiesel, with certain blending rate on volume premise, ought to be miscible in one another at the encompassing conditions and this as of now exists as blended powers, for example B5, B10 and so on., are sold at encompassing conditions and they are absolutely miscible. On the off chance that you need, you can test blending process tentatively at encompassing conditions and certain scope of low blending speed, for vitality sparing, at that point watch the ideal blending conditions. In the event that blending isn't acceptable you can rise blending rate or quest for certain added substances, for example surfactants, to achieve blending process.

MATERIALS AND METHODS

Castor is generally utilized as feedstocks for decrease of biodiesel,as its development needn't bother with significant expense and furthermore its concentrates contain 40-55% of oil in particular .Castor oil contains 80-90% of hydroxyl unsaturated fat, ricinoleic corrosive and about 10% of non-hydroxylated unsaturated fats, basically oleic corrosive and linoleic acids which causes a drawback for its utilization for biodiesel creation, since its thickness is around multiple times higher than the others. Ricinuscommunis, is ordinarily known as castor is a perenial blooming plant has a place with family euphorbiacae, these plants are local to tropical Africa and discovered to a great extent in the hot territories of the world.

Mahua oil got from mahua seed and castor oil is likewise extricated from castor seed. Mahua has a place tospecies of sapotaceae.It is an Indian tropical tree found over the northern part.Mahua oil is acquired from the piece of mahua seed (MadhucaIndica) which have 50-55% oil.The oil contains unsaturated fats like those in cooking oils as oleic corrosive, Linoleic acid.Stearic corrosive and palmitic corrosive. The particular gravity of mahua oil is 9.11% higher than diesel. The kinematic thickness of Mahua oil is 15.23 occasions more than diesel at temperature of 400 C .The kinematic consistency of mahua oil diminishes with increment in temperature upto 800 C and by expanding the proportion of diesel in fuel mixes.

The preparation of biodiesel from mixture of castor and mahuaoil is fundamentally done by transesterification process. This procedure should be possible in three phases as follows.

Pre-Process (Esterification)

1 liter of mixture of castor and mahuaoil was heated at 110°C to remove moisture content. After that the oil was cooled and 10gm of H_2SO_4 and 200 ml of methanol was added and mixed well. Then the oil mixture was placed in the biodiesel reactor and heated for 3hour maintaining the temperature 60-64 ^{0}C. After 3hour, the sample was cooled and collected in a separating funnel then on the next day the sample was filtered and the unreacted methanol was separated and the remaining product was transesterified. Esterification reaction is mostly used for reducing the FFA level of oil.

Main Process (Transesterification)

The esterified test was blended with 10g of KOH and 200 ml methanol. The blend was then warmed up to 3hour at 700°C in a biodiesel reactor with nonstop mixing .Then the sample was cooled and kept in an isolating channel. At that point on the following day we seen that two layers were framed and the upper layer which is the methyl ester was isolated from the lower layer which is the glycerol. Transesterification response is utilized for changing over unsaturated fat into unsaturated fat methyl esters. Transesterification can be completed by either corrosive impetus or antacid impetus. The term transesterification alludes to ester exchange response is transformation one ester to other. This incorporates all blends of association between monohydroxy liquor esters, mono and health food nuts of glycol mono di and triglycerides and the different esters of tetrahydroxy and higher liquor are conceivable. The ester – ester exchanges of materials expected for non-eatable mechanical uses are without a doubt getting progressively significant when applied to fats and oils ester – ester trade may improve physical properties since it changes acyl bunch course of action inside the parts of the blended triglycerides of fats and oils ester-ester exchanges might be influenced without impetus at high temperature at 1500C or more. Ester-ester exchange happens at quick and at less temperature by utilization of either corrosive or basic impetus. Ester trades continue aimlessly. This will bring about compositional changes; the greasy acyl bunches inside triglyceride to all the conceivable mix.

Post Process (Water Wash)

The methyl ester which is acquired is then water washed to evacuate the rest of the glycerol and debasements of arrangement. The methyl ester was blended in with water in 1:3 proportion and shaked well for 2 minutes and it was kept for 15 minutes. After that water was contracts debasements and the unadulterated methyl ester was gathered. This procedure was rehashed for 5-6 times. The gathered sample after water wash was warmed at 1100°C for 40-50 minutes then the biodiesel was collected.

Performance Test

The dual blended castor-mahua biodiesel is blended with diesel to get the desired fuel for testing in diesel engine. The prepared dual biodiesel of castor-mahuaB10 blend and castor biodiesel of B10 blend prepared by the prescribed method, were then tested in variable compression ratio engine shown in Fig.2, where there is a provision to change the compression ratio by changing clearance volume of the engine cylinder. The engine was started and run idle for 10 minutes. Now the compression ratio of the engine is set at 18. Then dual castor-mahua biodiesel B10 blend was poured in fuel tank and the engine was run with no load condition. The load was increased to 2kg by means of variac. Important performance parameters of the engine such as Brake Power (BP), Brake Thermal Efficiency and Specific Fuel Consumption (SFC) were obtained from a computer integrated with VCR engine. Gradually the engine load was increased to 4, 6 and 10 kg and corresponding values of performance parameters were recorded. This procedure was followed for B10 of castor biodiesel.

RESULTS AND DISCUSSION

The performance comparison of VCR engine using dual blend of castor-mahua B10, castor biodiesel of B10 blend and conventional diesel was shown in Fig.4-6. The key performance parameters which were taken into considerations were Brake Power (BP), Brake Thermal Efficiency and Specific Fuel Consumption (SFC). It is observed from the Fig. 4 and Fig. 5 that the Brake Power (BP) and Brake Thermal Efficiency of dual blended castor-mahua biodiesel blend B10 has been enhanced than castor biodiesel of same blend due to addition of equal quantity of mahua oil. For pure diesel, the values of Brake Power and Brake Thermal Efficiency are found to be highest among three fuels. This is due to more calorific value of diesel than other two fuels. However, at higher loads, the percentages increase in Brake Power and Brake Thermal Efficiency diminishing. The Specific Fuel Consumption (SFC) of dual blended castor-mahua biodiesel is slightly more than castor biodiesel. But that increase may be underestimated due to increase in more influential performance parameters like Brake Power and Brake Thermal Efficiency. Moreover there is no modification in engine which supports its usability as a fuel for internal combustion engine.

CONCLUSION

The performance tests of variable compression ratio diesel engine were conducted with diesel, castor biodiesel and dual blend of castor-mahuabiodiesel at different loads and constant speed 1500 rpm at fixed compression ratio 18. India being an agricultural country, the energy from bio sectors will be highly beneficial for both plantation as well as transportation. Thus dual blended biodiesel of castor and mahua oil will be a highly beneficial fuel in terms of both economy as well as fuel independence because these oils will be easily available as long as air and water are available in the earth. Theperformance results obtained due to combustion of dual blended castor-mahua biodiesel are giving comparable results without any engine modifications. Hence it can be considered as a good replacement for conventional diesel fuel at lower blends.

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Fig. 1.a. Castor Seed

Fig. 1.b. Mahua Seed

Fig.2. Biodiesel Reactor

Fig.3. Variable Compression Ratio Diesel Engine

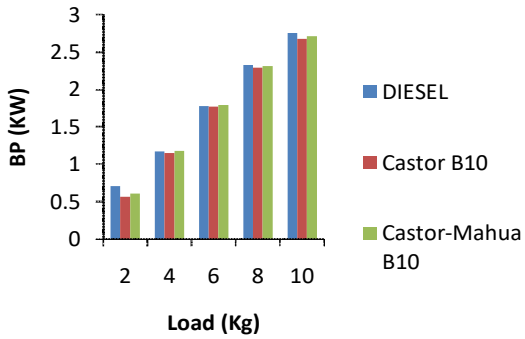

Fig.4. BP Vs Load of Three Different Fuels

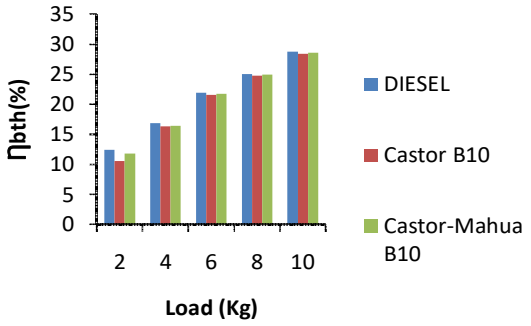

Fig.5. η_{bth} Vs Load of Three Different Fuels

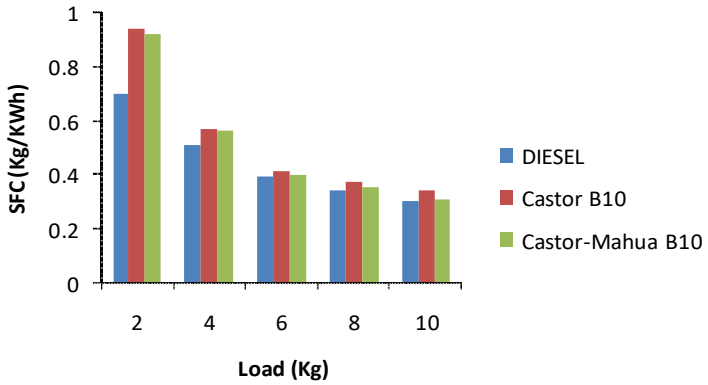

Fig.6. SFC Vs Load of Three Different Fuels

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RESEARCH ARTICLE

Structural and Dielectric Properties of Layered Structure Bismuth Oxide Ceramic $SrBi_2V_2O_9$

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ABSTRACT

The layered structure bismuth oxide ceramic $SrBi_2V_2O_9$ (SBV) belonging to the family of Aurivillius type was synthesized by solid state reaction method. The X-ray diffraction study reveals the orthorhombic crystal structure at room temperature. The dielectric properties (εr and tanδ) of sample at different frequencies in a wide range of temperature (25°-500°C) have been studied with an impedance analyzer. The studied sample has a dielectric anomaly at around 120°C.

Keywords: Solid state reaction; XRD; Dielectric Properties;

INTRODUCTION

The family of layered bismuth oxides ceramics was first reported by Aurivillius **[1],** while studying the Bi_2O_3-TiO_2 system which is now referred to as Aurivillius structure. Later on there are numbers of layered bismuth oxide materials from this family were reported which showed the ferroelectric properties **[2, 3].** The Bismuth Layer-Structured Ferroelectrics (BLSF) material is excellent candidate for nonvolatile Ferroelectric Random Access Memory (FRAM) in various commercial applications. There are various BLSF materials such as $SrBi_2Ta_2O_9$ (SBT), $SrBi_2Nb_2O_9$ (SBN), $SrBi_2$ $(TaNb)_2O_9$ (SBTN), have been obtained much attention because of their merits of fatigue resistance, lead free composition and FRAM characteristics [4]. Bismuth layered perovskites have high fatigue resistance that makes them capable to withstand 10^{12} erase or rewrite operations [5]. The general formula for BLSF is $Bi_2A_{m-1}B_mO_{m+3}$, where A= Bi, Pb, Na, K, Sr, Ba, like rare earths; B=Ti, Nb, Ta, Fe, Mo, W, Cr and m=1-6 [6]. The vanadium pent oxide (V_2O_5) was found to be an effective microstructure modifier and grain growth truncator for the $SrBi_2Nb_2O_9$ (SBN) ceramic. The materials $Bi_4V_2O_{11}$ is a layered structure bismuth oxide comes under Aurivillius family which shows three essential polymorphs phases like monoclinic, orthorhombic and tetragonal phase [7,8].

Realizing the importance of V_2O_5, we have synthesized and studied the structural, dielectric properties of $SrBi_2V_2O_9$ (SBV).

Experimental

The ceramic sample Strontium Bismuth Vanadium Oxide-$SrBi_2V_2O_9$ (SBV) was prepared by solid state reaction method using ingredients: $SrCO_3$, Bi_2O_3, V_2O_5 in a suitable stoichiometric proportion. The ingredients were thoroughly mixed by using an agate mortar and pestle in air-atmosphere and methanol. The mixed powders were calcined at an optimized temperature 600°C for 4h. The quality and formation of the calcined powder were checked through an X-ray diffraction (XRD) method at room temperature using CuK_α radiation (λ=1.54 Å).Then the calcined powder mixed with PVA (polyvinyl alcohol) as a binder was cold pressed into cylindrical pellets using a hydraulic press. The pellets were sintered at 650°C for 4h. The PVA which was used as binder to reduce the brittleness of the pellets, burnt out during sintering. In order to analyze the electrical properties of the sample, the sintered pellets were electroded with air-drying conducting silver paste. After electroding, the pellets were dried at 150°C for 4h to remove moisture, if any and then cooled to room temperature before taking any measurement. The dielectric measurements were carried out using a LCR meter (HIOKI Model 3532) in the frequency range of 10^2-10^6 Hz at different temperatures (25-450 °C).

RESULTS AND DISCUSSION

Structural Study

The room temperature XRD pattern of the studied sample SBV is shown in the Fig.1 All the reflection peaks of pattern were indexed in different crystal systems and unit cell configuration. An orthorhombic crystal system was calculated on the basis of good agreement between observed (obs) and calculated (cal) interplanar spacing d ($\sum\Delta d = d_{obs} - d_{cal}$ =minimum). The lattice parameters were refined using a standard computer program package "POWD" [9] and found to be a= 14.9706Å, b= 4.2677 Å, c= 10.4961 Å. The volume of the unit cell is V=670.59. The crystallite size (D) of the sample was determined by using Scherrer's equation [10] i.e., $D= k\lambda/(\beta_{1/2}\cos\theta_{hkl})$ and found to be 38 nm, where k= constant=0.89, λ=1.5405 Å, $\beta_{1/2}$=peak width of reflection at half intensity.

Dielectric Study

Fig. 2 shows the variation of dielectric constant (ε_r) and loss tangent (tanδ) with frequency at room temperature. It is observed that both the dielectric constant and the loss tangent decreases with rise in frequency at room temperature. At higher frequencies, the significant contribution to the dielectric constant is the electronic polarization where the other polarizations in the material become ineffective. A similar type of result has been reported by Kalaiselvi *et al* [11] by the study of SBVN [$Sr_{0.8}Bi_{2.2}(V_{0.2}Nb_{0.8})_2O_9$].

Fig. 3 shows the variation of dielectric constant (ε_r) with temperature at different frequencies. It is observed that ε_r increases gradually on increasing temperature to its maximum value (ε_{max}) and then decreases. A dielectric anomaly is observed around 120 °C. Above the temperature around 200 °C, the increase of ε_r may be due to space charge polarization which comes from mobility of ions and imperfection in the material. The dielectric anomaly which was observed at 120°C found to shift towards low temperature side with increase of frequency and this variation has been shown Fig 3 (inset). Similar trend of variation is observed in tanδ as in ε_r as a function of temperature also shown in Fig. 4. An anomaly in tanδ may be attributed to the dielectric relaxation in the material. The higher value tanδ at high temperature may be due to space charge polarization. Similar type of result has been reported by Yan *et al* [12,13] for different ceramics.

CONCLUSION

The layered structured bismuth oxides ceramics sample of $SrBi_2V_2O_9$ (SBV) was prepared by solid state reaction technique. The studied compound belongs to Aurivillius family and X-ray structural analysis exhibits the orthorhombic structure. The dielectric constant decreases with increase of frequency which is a general behaviors of dielectrics. The dielectric constant increases with increase in temperature and then decreases. Studies of the dielectric properties showed that the compound undergoes an anomaly at 120 ^oC and this anomaly shifted to lower temperature sides on increasing frequency.

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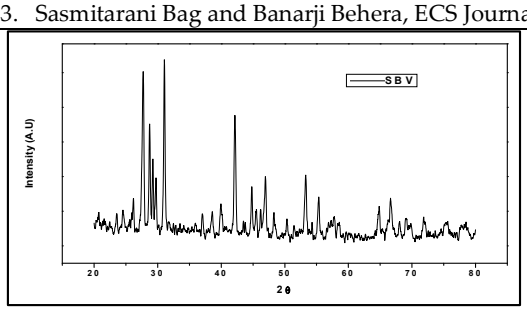

Fig.1 X-ray diffraction pattern of SBV at room temperature

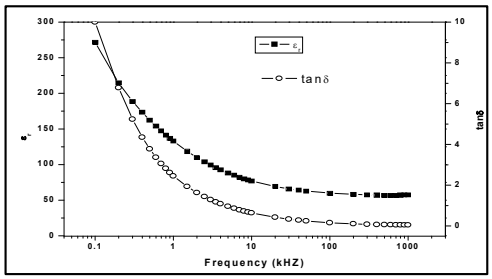

Fig. 2 Variation of ε_r and tanδ with different frequency at room temperature of SBV

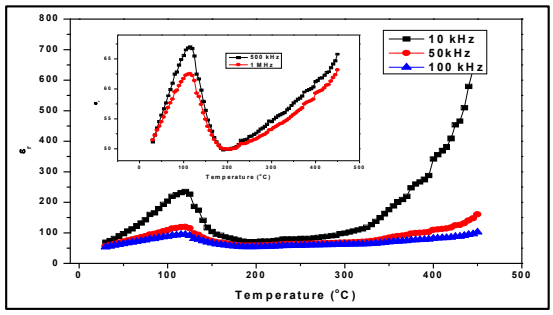

Fig. 3 Variation of ε_r as a function of temperature at different frequencies

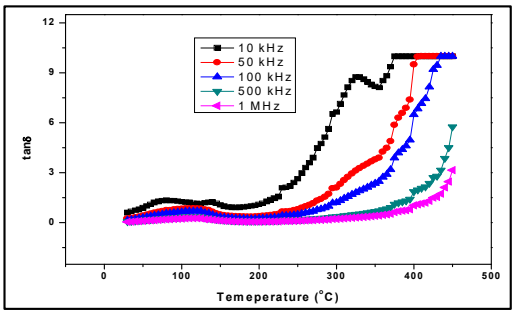

Fig: 4 Variation of tanδ as a function of temperature at different frequencies

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RESEARCH ARTICLE

Emission Characteristics of Diesel Engine with Mixed Biodiesel Blend of Castor and Mahua

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ABSTRACT

The depletion of petroleum fuels is a major concern now a day. The growth in automobile sector and population are the prime causes for it. Moreover the emission from vehicles that uses petroleum fuels such as petrol, diesel and kerosene possess a threat to the environment and mankind. The major gases coming out from the vehicle emission such as Carbon Monoxide (CO), Carbon Dioxide (CO_2), Oxides of Nitrogen (NOx), Hydro Carbon (HC), Particulate Matter (PM) are polluting atmosphere to great extent. Many researchers have proposed several ways of reducing pollution by using alternate energy sources. Use of biodiesel as a liquid alternate fuel is one of the biggest achievement so far. As the name suggests, it can be produced from biofuels and has similar properties with conventional diesel fuel. The wide availability of plant such as karanja, Mahua, Sunflower, Kusuma, jatropha, Castor is favourable for biodiesel production. Researchers are going in favour of different non edible oil sources because they are non-consumable for human being. Characteristics of these oils need to be carefully studied before proceeding for biodiesel production. However the use of biodiesel as fuel for vehicles decreases the performance slightly due to less calorific value as compared to conventional diesel and petrol. But on the other hand, there is a significant reduction in pollution level as reported by different researchers. In this work, a mixed biodiesel blend of Mahua and castor has been prepared and used as an alternate fuel to run a diesel engine. The results obtained give a reduction in emission gases as compared to castor biodiesel of same blend.

Keywords : Emission, Diesel Engine, Biodiesel, Blend, Castor, Mahua

INTRODUCTION

Biodiesel is an alternative fuel for diesel which is derived from either plants and plant product or animals. It is produced by chemically reacting a vegetable oil or animal fat with an alcohol such as methanol or ethanol. That chemical reaction which converts a vegetable oil or animal fat to biodiesel is called "transesterification".Ghaly et al. [1] told that the research on the production of biodiesel has increased significantly in recent years because of the need for an alternative fuel with low toxicity and renewability.Deepanraj et al. [2] described that the lower blends of biodiesel increased the brake thermal efficiency and reduced the fuel consumption. In addition to that, it was reported that biodiesel blends produce less engine emission than conventional diesel fuel.Mahalingam et al. [3] carried out their research on emission analysis of a diesel engine by using biodiesel blends of mahua and alcohol. Rathore et al. [4] carried out experimental analysis on performance and emission of modified diesel engine by using mixed biofuel blends of coconut and karanja. Bajpai and Das [5] did their experimental work on running engine with different biodiesel blends of Jatropha, Karanja and Castor. They found lower blends were giving the performance result close to diesel oil. Jena et al. [6] carried out their investigation on biodiesel preparation from mixture of mahua and simarouba oil and reported comparable fuel properties with diesel. Foroutan et al. [7] produced biodiesel from waste edible oils in the transesterification process by using nano catalyst of magnesium and calcium. Despite so many works on biodiesel, much work has not been done with mixed biofuel blends.

In this work, the mixture of two different oils i.e. castor and mahua were mixed together in equal proportion and was used to prepare biodiesel. The prepared biodiesel was used to run a diesel engine and exhaust gases coming out of the tail pipe was analysed to determine the percentage of exhaust gases. The engine was also run with prepared castor biodiesel of same blend separately. A detailed comparison of the constituent of the engine emission was made in both cases.

MATERIALS AND METHODS

Castor is widely used feedstock for reduction of biodiesel,as its cultivation does not need high inputs and also its extracts contain 40-55% of oil only [8] .Castor oil contains 80-90% of hydroxyl fatty acid, ricinoleic acid and about 10% of non-hydroxylated fatty acids, mainly oleic acid and linoleic acids which causes a disadvantage for its use for biodiesel production.Mahua belongs tospecies of sapotaceae.It is an Indian tropical tree found across the northern part.Mahua oil is obtained from the kernel of mahua seed (MadhucaIndica) which have 50-55% oil.The specific gravity of mahua oil is 9.11% higher than diesel. Therefore, the mixing of 50% of castor oil with 50% of mahua oil is carried out at room temperature for better result. And also it is a new way of making biodiesel by adding or blending these two different oils together. The final product of mixing should be homogeneous.

Preparation of Biodiesel

1 liter of mixture of castor and mahua oil in equal proportion (1:1) was taken and heated at 110^0 C to remove moisture content. Then esterification process was carried out by heating in a biodiesel reactor as shown in Fig.1 in the presence of 10 gm of H_2SO4 with 200 ml of methanol. After 3hours of heating the sample was cooled and collected in a separating funnel. The unreacted methanol was separated and the remaining product was transesterified in the presence of 10g of KOH and 200 ml methanol solution by heating in a biodiesel reactor at 70^oC. After 3 hours of continuous heating with stirring, the sample was collected in a separating funnel. After keeping in funnel for some times, the two different layers were formed. The upper layer was methyl ester and lower layer was known as glycerol. The required methyl ester was washed several times with water until no soap bubbles were observed inside methyl ester. This is the required biodiesel which is mixed with diesel fuel to get desired blending. A blend of Castor-Mahua mixed biodiesel B10 which can be written asD90C5M5 (i.e 90% diesel, 5% Castor and 5% Mahua) was used as fuel to run a diesel engine. The exhaust gases emitted in the tail pipe was tested by using exhaust gas analyser.

Emission Test

The exhaust gas from diesel engine was analysed by means of gas analyser in pollution testing apparatus shown in Fig.2, which was integrated with the engine. The probe of the analyser was inserted in the exhaust pipe of the engine to sense the exhaust gas. The composition of exhaust gases which mainly consists four major pollutants such as CO, CO_2, $NO_x$and HC were recorded during testing of different blends of castor biodiesel.

RESULT AND DISCUSSION

Carbon Monoxide (CO) emission

The Carbon Monoxide (CO) content of the diesel engine emission due to combustion of Castor-Mahua mixed biodiesel B10 (D90C5M5) is presented in Table 1 and a comparison of CO percentage with diesel and castor biodiesel is shown in Fig.3.The percentage of CO comparison between three different fuels indicate that CO content is less for biodiesel B10 (D90C5M5) than conventional diesel and castor biodiesel of same blend. The result of carbon monoxide presence in the engine emission is due to incomplete combustion of fuel. Due to the addition of extra oxygen molecule in Castor-Mahua mixed biodiesel (D90C5M5), it results in better combustion and hence less CO content.

Carbon Dioxide (CO_2) emission

The Carbon Dioxide (CO_2) content of the diesel engine emission due to combustion of Castor-Mahua mixed biodiesel B10 (D90C5M5) is presented in Table 2 and graph is plotted by taking different loads on the engine as shown in Fig.4. It is observed from the results that CO_2 percentage for B10 (D90C5M5) is slightly more than castor biodiesel of B10 blend and diesel fuel.

Hydrocarbon (HC) emission

The Hydrocarbon (HC) content of the diesel engine emission due to combustion of Castor-Mahua mixed biodiesel B10 (D90C5M5) is presented in Table-3 and a comparison of HC content expressed in parts per million (PPM) between three different fuels are shown in Fig.5.It is quite apparent that the hydrocarbon content for mixed biodiesel B10 (D90C5M5) reduces significantly as compared to diesel and also with castor biodiesel. The reason is due to complete combustion of fuel which results in left unburnt hydrocarbon due to rich oxygenated fuel.

Oxides of Nitrogen (NOx) emission

The NOx content of the diesel engine emission due to combustion of Castor-Mahua mixed biodiesel B10 (D90C5M5) is presented in Table 4.A comparison of NOx quantity is made with diesel and castor biodiesel as shown in Fig.6. It is observed that NOx emission increases with increase in load. The result also reveals that the NOx content in emission enhances for castor biodiesel and mixed biodiesel (D90C5M5). The reason may be due to higher combustion chamber temperature of engine when it uses biodiesel as biodiesel is more oxygenated in nature. The value of NOx quantity increases slightly for Biodiesel B10 (D90C5M5) than castor biodiesel B10 blend. However at higher load that increment is very less.

CONCLUSION

The emission characteristics of single cylinder, four stroke diesel engine fuelled with mixed biodiesel blends of castor and mahua oil have been investigated. Mixed Biodiesel blend of B10 (D90C5M5) has shown reduction in toxic pollutants like HC and CO than diesel and castor biodiesel without any engine modification. CO_2 and NOx emissions wereslightly more for the biodiesel blends as compared to diesel.

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Fig.1. Biodiesel reactor

Fig.2. Pollution testing apparatus

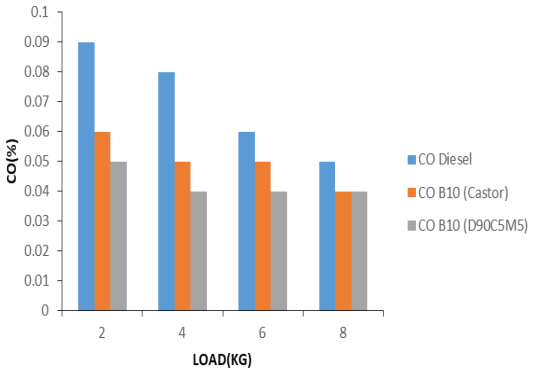

Fig.3. CO Vs Load for three different fuels

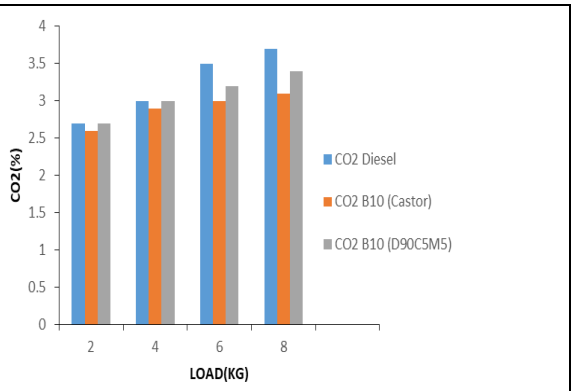

Fig.4.CO_2Vs Load for three different fuels

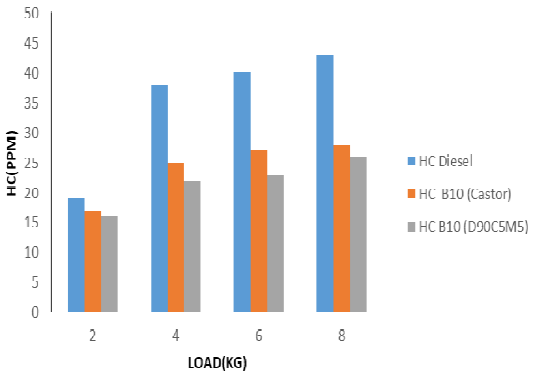

Fig.5. HCVs Load for three different fuels

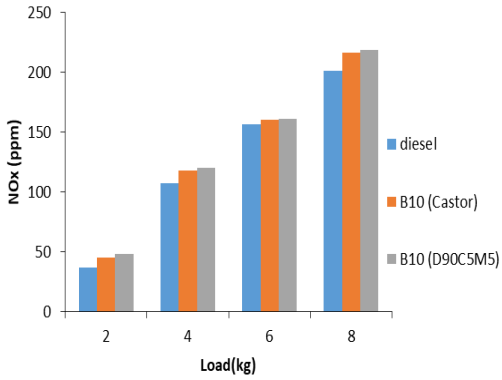

Fig.6. NOxVs Load for three different fuels

Table 1.CO content in the engine emission of fuels

Load	CO (%) Diesel	CO (%) B10 (Castor)	CO (%) B10 (D90C5M5)
2	0.09	0.06	0.05
4	0.08	0.05	0.04
6	0.06	0.05	0.04
8	0.05	0.04	0.04

Table 2.CO_2 content in the engine emission of fuels

LOAD	CO_2 (%) Diesel	CO_2 (%) B10 (Castor)	CO_2 (%) B10 (D90C5M5)
2	2.7	2.6	2.7
4	3	2.9	3
6	3.5	3	3.2
8	3.7	3.1	3.4

Table 3.HC content in the engine emission of fuels

Load	HC (PPM)	HC (PPM)	HC (PPM)
	Diesel	B10 (Castor)	B10 (D90C5M5)
2	19	17	16
4	38	25	22
6	40	27	23
8	43	28	26

Table 4.NOx content in the engine emission of fuels

LOAD	NOx (ppm)	NOx (ppm)	NOx (ppm)
	diesel	B10 (Castor)	B10 (D90C5M5)
2	37	45	48
4	107	118	120
6	156	160	161
8	201	216	218

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RESEARCH ARTICLE

Tunable Metamaterial Antenna

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ABSTRACT

Metamaterials are composite materials whose material properties (acoustic, electrical, magnetic, or optical, etc.) are determined by their constituent structural materials, particularly the unit cells. Metamaterial technolgy aims to redefine the the boundaries of materials science. These materials give excellent design versatility in the field of electromagnetic science and beyond, with their tunability under external stimuli. Metamaterials are constructed to shape a single, two or three-dimensional volume by embedding sub-wavelengths inclusions into a host medium .Such inclusions are similar to artificial molecules that can be designed to achieve the desired response of bulk material. Through this way, the metamaterial gains its properties not from its composition, but from its structure. The split-ring resonator exhibits diamagnetic properties over a small bandwidth but no magnetic materials are required for its construction. This researchinvolves electromagnetic metamaterials operating at microwave frequencies (C microwave band, nominally 4.0 GHz to 8.0 GHz) and their application to the slotted waveguide antenna stiffened structure (SWASS). The sub-wavelength inclusions take the form of electronic circuits designed using conventional printed circuit board (PCB) and lithographic techniques along with traditional circuit elements such as inductors, capacitors and resistors. The inclusions are arranged into periodic unit cells with millimetre dimensions. The bulk material response of the metamaterial will be definedvia its effective material properties such as the electrical permittivity and magnetic permeability.

Keywords: Metamaterials, slotted waveguide antenna stiffened structure (SWASS), permittivity, permeability, unit cell.

INTRODUCTION

An artificial structural feature is a metamaterial structure designed to achieve advantageous and unsual electromagneic and provide a new prospective in the understanding of material through their custom dielectric properties and tunable responses. The launch of this new field is marked by the famous paper by John Pendry [1], published in the year 2000 after Veselago's visionary proposal on a similar topic had been neglected for over 30

years. Within 10 years of Pendry's paper, metamaterials became a breakthrough technology due to their potential for clocking and light manipulation [2-6]. With the development of this new technology, more and more uses in telecommunications, sensing, aerospace, the optics (tera Hertz and infrared), and health-care have emerged. Metamaterials also demonstrate great potential for military and defense use in addition to industrial applications. The Defense Advanced Research Projects Agency (DARPA), the North Atlantic Threaty Organization (NATO), and major defense companies worldwide pay close attention to devolving this field. Devoloving in this area has become a major focus of attention.Metamaterials can revolutionize how the electromagnetic spectrum is manipulated. There are numerous interesting new ways to use the literature to build on the exotic properties of metamaterials. However, very few useful applications for killing have evolved mainly because of the narrow band and the high loss of the current metamaterial structures.This work aims to tackle the bandwidth limitation by combining electronically tunable elements with a unit cell design that permits control of the proposed metamaterial over the entire C microwave band. Within this new metamaterial unit cell, stronglylocalized electromagnetic fields and current are used to improve the performance of the slotted waveguide antenna stiffened structure (SWASS).

Development and Future

As highlighted in the comprehensive review by Kadic et al. titled *Metamaterials beyond electromagnetism* points out, the metamaterial concept also applies to thermodynamics and classical mechanics (including elastostatics, elastodynamics, acoustics, and fluid dynamics) [7]. Many related areas are envisaged to grow quickly as optical metamaterials and electromagnetic metamaterials evolve and flourish.There is no doubt that the tread towards the next stage of metamaterial development will be controllable metamaterial, on which smart structures and smart skin are built.Through the path, bullet trains and recreational vehicles (RVs) will obtain best signals, using these materials and technologies. In the future, metamaterial design will be more challenging than a cross -disciplinary approach and a multi-model on the proof-of- concept, product and device requirements. At the microwave frequencies (C microwave band, nominally 4.0 GHz to 8.0 GHz), the proposed electromagnetic metamarials willl function.

Metamaterials are novel synthetic materials that exhibits unique properties not found in nature. Metamaterial and metasurface does not comes under classical periodic structures i.e. photonic band gap structure (PBG) or frequency-selective-surfaces (FSS), rather than a particular class of metamaterial is characterized with double-negataive (DNG) materials. Such material exhibits property of negative permittivity and permeability in a given frequency band.

Originally, the surface vision of metamaterial is name as metafilm. So, metafilm is referred as metasurface, which is the surface distribution of large number of electrically small scatterers (e.g., metallic rings and rods, or spherical magneto-dielectric particles) [8]. The small scatterers can be arranged in a periodic manner throughout the region to obtain a bulk electromagnetic behaviour. It is not necessary that the constituent of metafilm i.e. the small scatters to be of zero thickness. Electric and magnetic polarizabilities define the behaviour of metafilm. Three-dimensional metamaterials can be extended by placing the scatterers in a two-dimensional arrangement over a surface. Figure 1 shows an arrangement of unit cells in a metascreen.

Metasurface is characterized with a cermet topology. It refers to an array of isolated scatterers called metafilms. Metascreen is the fishnet structure of metasurface. These are characterized with periodically spaced apertures relative to impenetrable surface.

For example, a grating of parallel conducting wires behaves like a metafilm in the direction perpendicular to the wires' axes, but like a metascreen in the direction along these axes.

Characteristics

a. Compact size
b. Low profile
c. Conformal

d. Multiband or broad-band
e. Low frequency
f. Low SAR

Advantages

i. It takes less physical space to do full 3-D structure and offer the possibility of reduced loss.
ii. Metamaterial will provide miniaturization of the antenna with desired frequency along with SAR reduction.
iii. A slab of DNG material, with flat faces, could act like a lens and would have a better performance than other diffraction-limited systems, such as a conventional convex lens made with a DPS material, for instance glass.
iv. The inductive and capacititve elements of both metasurface produces high transmission with variable phase characteristics.

Applications

The theory of metafilm produce some potential application which includes: (a) controllable "smart" surfaces, (b) miniaturized cavities, (c) new wave guiding structures, (d) switches, and (e) bio-medical devices.

The use of anisotropic scatterers to make up a metafilm can be used to achieve a number of useful results not possible with isotropic metasurfaces. One of the more interesting aspects of bulk metamaterials is the ability to engineer anisotropic behavior into them. In fact, this is the idea behind socalled “cloaking” materials, which has generated so much media interest. The cloaking concept is to design a specific anisotropic behavior into a metamaterial in such a way as to cause electromagnetic energy to propagate or bend around an object that is covered with it. If the anisotropic materials are correctly designed, the coated object will neither scatter nor absorb energy, and hence it appears to the electromagnetic (EM) fields as if the object is not present.

It controls the wavefront of EM waves by imparting local, gradient phase shift to the incoming waves, which leads to a generalization of the ancient laws of reflection and refraction. In this way metasurfaces can be made as a planar lens, vortex generator, beam deflector, axion and so on.

Metasurfaces can also find applications in electromagnetic absorbers, polarization converters and spectrum filters.

CONCLUSION

In academic research and the industry, we examined the development of metamaterial technology. Control and manipulation of electromagnetic, optic, and acoustic waves distinguishes metamaterials from traditional materials.Metamaterials should be able to change transmission, reflection, absorption, and steering beam direction, heat conduction control, and more with their tunability. Even without human intervention they wouldable to sense and react. Metamaterials have reshaped the science of matter. It is time we rethought their abilities.

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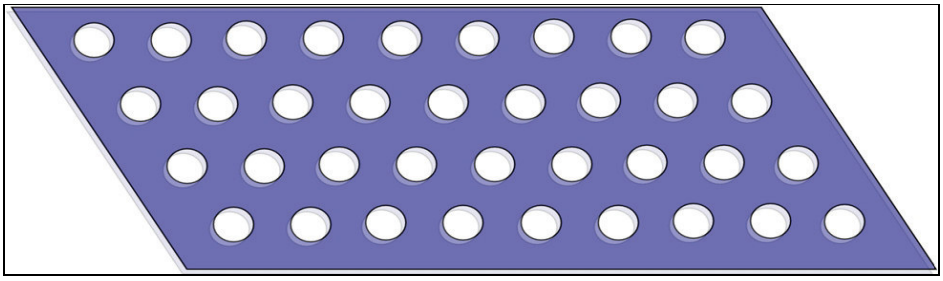

Figure 1. A metascreen

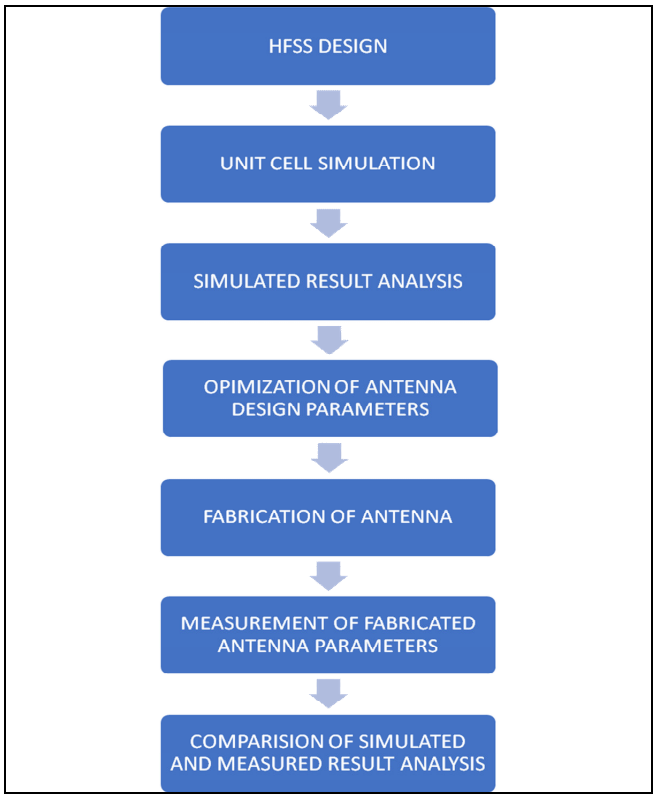

Figure 2. Flow chart of metamaterial antenna design

Proposed Methodology

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RESEARCH ARTICLE

Identification of Potential Therapeutic Phytochemicals of Bael (*Aegle marmelos*) against Emerging Human Pathogen *Helicobacter pylori:* A Novel Hierarchical *In silico* Approach

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ABSTRACT

Colonization of *Helicobacter pylori* in human gastric epithelial tissue and mucus membrane is associated with gastritis. There is also evidence that, it causes peptic ulcers, duodenal ulcers and chronic gastritis. In developing countries, prevalence of *H. pylori* infection is more than 90% and is about 50% infected adult cases in industrialized countries. Hence, array of new drugs development for the treatment of *H. pylori* infection is great concern. Urease is a key enzyme in *H. pylori* metabolism and virulence and it also plays a major role during colonization of this pathogen with gastric mucosa membrane. So, Urease may be a potential target for dug designing and vaccine development. In this study, we retrieved *H. pylori* urease structure from PDB and used it as a drug target protein. Phytochemicals have been used as drugs since ancestral time period. One of the potent phytochemicals of Bael (*Aegle marmelos)* is lupeol. Structure of the lupeol was retrieved from Pubchem and docking was performed by using Swissdock softwares. Swissdock is a web server specially designed to carrying out protein-ligand docking simulations. In our docking study, we found phytochemical lupeol from Bael is effective against urease enzyme of *H. pylori.* We also concluded that, in silico docking study is also a better approach to check the utility of any phytochemical as a drug than in –vivo and in-vitro study.

Key words: Phytochemical, Swissdock, Bael (*Aegle marmelos*), *Helicobacter pylori,* Lupeol, Urease

INTRODUCTION

Helicobacter pylori was formerly known *Campylobacter pylori* is associated with gastritis, peptic ulcers, duodenal ulcers and chronic gastritis. It colonizes gastric epithelial tissue ad mucus membrane. It has been also reported that, *H. pylori* is carcinogenic to human [1]. Combination of bismuth with antibiotics and proton-pump inhibitor with

antibiotics are most commonly used antimicrobial therapy against *H. pylori* infections [2]. Transmission of *H. pylori* occurs through the oral-oral and faecal-oral routes [3]. The most likely transmission route is person to person. It is a gram-negative, spiral shaped microaerophilic bacteria and optimal growth occurs in presence of 5-15% oxygen. Optimum pH range for growth of *Helicobacter pylori* is 4.5 to 9 and optimum temperature range is 30 to 37°C. Habitat for the growth of this bacteria is human stomach. It has been also isolated from domestic animals like cat [4]. Epidemiological studies have been proved that, transmission occurs through food and water. Consumption of uncooked vegetables that had been irrigated with water contaminated with untreated sewage was associated with *H. pylori* infection in Chile, South America etc. There are various lab diagnosis methods available for the detection of *Helicobacter pylori* infection. Among these diagnosis methods, detection of urease enzyme in infected person's stomach is a confirmatory test because *H. pylori* is the only organism that expresses urease. This urease enzyme helps in colonization of *H. pylori* with gastric mucosa of humans [5]. Urease (urea amidohydrolase: EC 3.5.1.5) catalyzes hydrolysis of urea to produce ammonia and carbamate, which subsequently produces ammonia and carbonic acid. It is a multisubunit metalloenzyme.

Bael (*Aegle marmelos)* is one of the most popular traditional medicinal plant in Indian origin. It is a spiritual, religious and medicinal plant found in Asian countries like Bangladesh, Indonesia, China, etc. It contains various phytochemical like alkaloid, tannins, essential oils, resins and gums etc. Following is the taxonomical classification of Bael (*Aegle marmelos)* [6]-

Taxonomy

Kingdom	:	Plantae
Order	:	Sapindales
Family	:	Rutaceae
Sub family	:	Aurantioideae
Genus	:	Aegle
Species	:	A. marmelos

Broad therapeutic application of Bael (*Aegle marmelos)* includes antidiarrheal, antifungal, antidiabetic, analgesic, anti-inflammatory, antipyretic, antimicrobial, antiulcer, antitubercular, antidandruff and antiviral activity etc [7,8]. Lupeol is one of the most active ingredients present in Bael. The other nutritional constituents present in Bael fruits are water, sugar, protein, fiber, fat, calcium, phosphorus, potassium, Iron and vitamins (Vit A, Vit B, Vit C and Riboflavin). The various polysaccharides present in Bael are galactose, arabinose, uronic acid etc. Carotenoids are chief pigments responsible for imparting pale yellow colour to fruit. Over the last few years, researchers are aimed to identify and validate phytochemicals for the treatment of many emerging diseases. These phytochemicals are easily available, cost effective and having less side effects than conventional drugs.

In this present study, molecular docking was performed by using Swissdock softwares. Docking is a method which predicts the preferred orientation of one molecule to a second when bound to each other to form a stable complex. Knowledge of the preferred orientation in turn may be used to predict the strength of association or binding affinity between two molecules. Docking is frequently used to predict the binding orientation of small molecule (ligand) drug candidates to their protein targets in order to in turn predict the affinity and activity of the small molecule [9, 10].

MATERIAL AND METHODS

Protein structure (PDB ID-3cxn) files of *Helicobacter pylori* urease was retrieved from PDB site containing resolution about 1.55A^0 and used as a drug target protein. Phytochemicals of Bael ((*Aegle marmelos)* lupeol structure was also retrieved from Pubchem. Docking study was performed by using Swissdock softwares. The value was obtained in terms ΔG Kcal/mol. Energy value is inversely proportional to the affinity of the molecule to be used as a drug. So,

lesser the (ΔG) of phytochemical molecule indicates higher affinity of that phytochemical as a drug. In online swissdock software, protein urease was browsed in it. The selected molecule (lupeol phytochemical) was docked at different sites of target urease protein. After completion of docking, the result was obtained at provided email ID. The result was analyzed at the link provided in the email. UCSF chimera was used to find the predicted binding modes.

RESULTS AND DISCUSSION

From this Swissdock molecular docking studies, we found good ΔG Kcal/mol value with lupeol. The ΔG Kcal/mol value was about -5.55. With Swissdock molecular docking system, the result was obtained in terms of full fitness. This lesser value of ΔG indicates, the successful approach of phytochemical lupeol from Bael (*Aegle marmelos)* as a drug against emerging carcinogenic pathogen *Helicobacter pylori* urease enzyme. Lupeol can be a potent phytochemical for the treatment of gastritis, peptic ulcers, duodenal ulcers and chronic gastritis.

CONCLUSION

This study suggest that, Lupeol, phytochemicals from Bael ((*Aegle marmelos)* can be used as a potent molecule against *Helicobacter pylori.* It can be used as a basic approach to design a drug against this emerging carcinogenic pathogen. Further in- vitro and in-vivo studies is required for the extension studies of this approach. Use of bioinformatics tool and computational biology for the drug design is a better approach to limit the time and cost that is required for the in-vitro and in-vivo drug designing studies.

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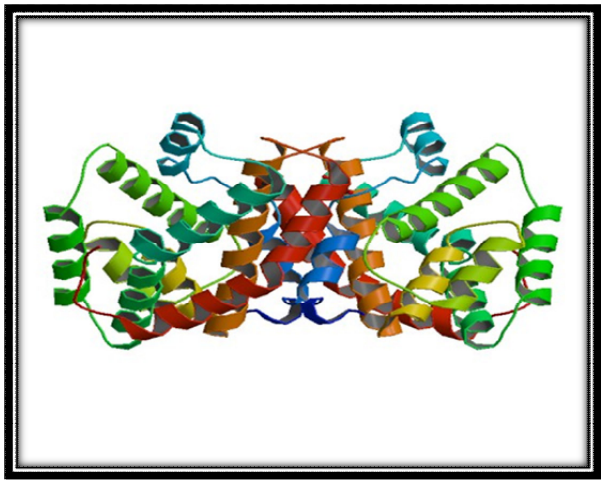

Figure 1- PDB ID-3CXN (Protein urease from *H. pylori*)

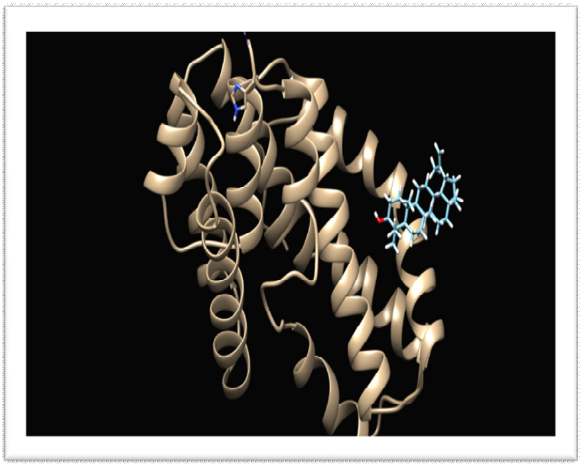

Figure 2- Docking of 3cxn (Urease) of *H. pylori* with Swissdock viewed in UCSF chimera

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RESEARCH ARTICLE

In silico Molecular Docking Analysis of Phytochemicals from *Curcuma longa* (Turmeric) against Aminopeptidase Nof *Escherichia coli* causing Infections in Urinary Tract (UTI)

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ABSTRACT

Phytochemicals are non-nutritive compounds obtained from plants through primary or secondary metabolism.Wound healing is a complex process of recovering the forms and functions of injured tissues. The process is tightly regulated by multiple growth factors and cytokines released at the wound site. Any alterations that disrupt the healing processes would worsen the tissue damage and prolong repair process. Various conditions may contribute to impaired wound healing, including infections, underlying diseases and medications. Numerous studies on the potential of natural products with anti-inflammatory, antioxidant, antibacterial and pro-collagen synthesis properties as wound healing agents have been performed. Their medicinal properties can be contributed by the content of bioactive phytochemical constituents such as alkaloids, essential oils, flavonoids, tannins, saponins, and phenolic compounds in the natural products. The plant extract contains different phytochemicals. It has been reported that *Curcuma longa* plant extract is used to cure UTIs.Urinary tract infection (UTI) is a condition in which the urinary tract is infected with a pathogen causing inflammation which is a widespread, difficult and rarely life threatening condition. UTI is caused by *Pseudomonas aeruginosa.* Turmeric (*Curcuma longa*), a commonly used spice throughout the world, has been shown to exhibit anti-inflammatory, antimicrobial, antioxidant, and anti-neoplastic properties. The molecular docking of the phytochemicals with the enzyme was studied using Swissdock. In our docking study, we found phytochemical Aminopeptidase Nfrom Turmeric is effective againstAminopeptidase N enzyme of *E. coli.* We also concluded that, in silico docking study is also a better approach to check the utility of any phytochemical as a drug than in –vivo and in-vitro study.

Key words: phytochemical, Swissdock, *Curcuma longa*, *Escherichia coli*

INTRODUCTION

In former days, life was natural, steady, difficult at times but healthy. Now, in modern times, life is fast paced, comfortable, ready made, stressful and unhealthy. Changing work condition, environment, less physical activity, sedentary jobs, comfortable but stressful life and bad food habits has exposed us to some dangerous health problems like various infections, blood pressure, diabetes, obesity etc. A little caution, small changes in lifestyle and care if taken, we can prevent these lifestyle related diseases from increasing.Antimicrobial properties of medicinal plants are being increasingly reported from different parts of the world. Plants are very significant to human, because they have several dynamic constituents which are precursor to synthesize many drug. India has a rich flora that is widely distributed throughout the country. Herbal medicines are basis of treatment and cure variety of diseases. Plant based drugs were commonly used in India and China. This study examines effectiveness of Curcumin is a bio-active substance from turmeric. Owing to antimicrobial properties, its prospect as an antibacterial agent is currently under focus. The world health organization (WHO) has estimated that about 80% of the population living in the developing countries depends tremendously on traditional medicine for their primary health needs. More than half of the world's population still depends exclusively on medicinal plants, and plants offer the active ingredients of most traditional medical products (Kumar and Navaratnam, 2013).Pharmacological studies have shown that intake of fruits and vegetables as well as other plant products are helpful to diminish the risks associated with diseases. According to World Health Organization, medicinal plants would be the meritorious source in obtaining different types of drugs. More than 80% of individuals from developed countries depend on conventional medicines, whose components are derived from plants sources. This suggests that plants would be a source of immense potentials and could be investigated thoroughly for understand their therapeutic properties, safety and efficiency. Various medicinal plants have been used for years on a regularbasis to improve the life quality of people all around the world .[2]

India has a rich history of using plants for medicinal purposes. Turmeric (*Curcuma longa* L.) is a medicinal plant extensively used in Ayurveda, Unani and Siddha medicine as home remedy for various diseases.It is used as a main ingredient of cooking in Asian countries. Because of its yellow colour it is also employed as a dye. It has been widely investigated and found to have many applications. Important applications are in cancer, diabetes, asthma, anemia and intestinal disorders. In dermatology, it has wonderful wound healing activity. Furthermore, it improves skin complexion. It has antioxidant, anti-inflammatory, antiviral, antibacterial and antiseptic properties (Satoskar et al., 1986; Ramirez-Bosca et al., 1995; Khiljee et al., 2011)*C. longa L.*, botanically related to ginger belongs to the Zingiberaceae family. Broad therapeutic application of Turmeric(*Curcuma longa)* includes antidiarrheal, antifungal, antidiabetic, analgesic, anti-inflammatory, antipyretic, antimicrobial, antiulcer, antitubercular, antidandruff and antiviral activity etc.

Urinary tract infection (UTI) was mostly caused by Gram negative (GN) bacteria, predominately by *E.coli.* UTIs are among the most common bacterial infectious diseases encountered in clinical practice and account for significant morbidity and high medical costs. *Escherichia coli* is the most predominant pathogen causing 80 to 90% of community-acquired UTIs and more than 30% of nosocomially acquired UTIs. Recurrent UTIs (RUTIs) are reported in 16–25% of women within six months and in 40–50% of women within one year of an UTI episode, and thus pose a major clinical problem. We previously showed that up to 77% of RUTIs are caused by *E. coli* identical to the primary infecting *E. coli,* but characteristics of *E. coli.* associated with persistence or relapse of UTI remain poorly defined. *E. coli* can be separated in four phylogenetic groups (A, B1, B2 and D) that appear to have different ecological niches and propensity to cause disease. It is so far unknown whether there is an association between phylogenetic groups and *E. coli* causing RUTIs.

Pathogenic microorganisms can cause number of diseases by their harmful quality of invasiveness and toxic character. Synthetic antibiotics used against them can cause oxidative stress along with damage to the DNA, proteins and lipids in human cells, the consequences of which could be life threatening at times. Due to the presence of phytochemicals and antioxidants, plants can pave a way for development of antimicrobial drug[3] *E. coli* can invade

and replicate within the murine bladder forming biofilm-like intracellular bacterial communities (IBCs) and establish quiescent intracellular reservoirs that may represent stable reservoirs for RUTI. No antibiotics have proven efficient in eradicating the UPEC reservoirs in the bladder in mice. Exfoliated IBCs and filamentous *E. coli* have been detected in urine from women with acute uncomplicated cystitis indicating that this pathogenic pathway may occur in women with UTIs.

We performed docking study using software namely Swissdock and database PubChem for getting structures of chemical constituents. Computational Biology and bioinformatics have the potential not only of speeding up the drug discovery process thus reducing the costs, but also of changing the way drugs are designed. In the field of molecular modeling, docking is a method which predicts the preferred orientation of one molecule to a second when bound to each other to form a stable complex. Knowledge of the preferred orientation in turn may be used to predict the strength of association or binding affinity between two molecules. Docking is frequently used to predict the binding orientation of small molecule drug candidates to their protein targets in order to in turn predict the affinity and activity of the small molecule.

MATERIALS AND METHODS

Software used

Swissdock softwarewas used for analysis. The software utilizes molecular level machine learning techniques to predict the level of molecular interaction.

List of phytochemicals

Phytochemicals are produced by plants as secondary metabolites to protect them from predators. The potential threats to plants include bacteria, viruses, fungi etc. When these plants or their parts are consumed by humans these phytochemicals fight off threats to health. Some phytochemicals have been used as poisons and others as traditional medicine. Published works have reported *Curcuma longa* to contain Desmethoxycurcumin, flavonoids, terpenoids, tannis, bisDesmethoxycurcumin, phlobatannis, and coumarin etc. It has already been established that *Curcuma longa* plant belonging to family Zingiberaceae has potential to help controlling UTI. This work is focused on identification of the particular phytochemicals responsible for inhibiting and controlling of UTI.

It is reportedthat Turmeric contains many phytochemicals (secondary metabolites) like alkaloids, tannins, steroids, saponin, flavonoids and many others. Phytochemicals are the non-nutritive chemical constituents of plants which help to protect the plant for defence and prevent them from being infected by diseases. Apart from the defensive property these phytochemicals have on the plants, they also protect humans against variety of diseases.

Enzyme found in *E. coli*

It has been reported that UTI can cause as a result of *E. coli* infestation. Various metabolic cycles have been seen in the bacterial life cycle for its survival. These metabolic cycles are regulated by different enzymes. Brenda enzyme database was used to identify and list different enzymes found in *E. coli* bacteria. It has been found that Aminopeptidase N enzyme in complex with Beta Alanine (protein database code 4xn9) is involved in some metabolism and very crucial for survival of the particular microbe.

Molecular docking

Molecular docking method has been used to identify the phytochemical from the plant extract, that act as a ligand and form a strong covalent bond with the bacterial protein to successfully inhibit the microbe. The Swissdock software was used for identifying molecular interaction and perform molecular docking. In this process first the sdf

files for the phytochemicals found in the *Curcuma longa* plant were downloaded from the website (refer). The protein database code of the Aminopeptidase N enzyme was identified from the website (refer).

RESULTS AND DISCUSSION

From this Swissdock molecular docking studies, we found good ΔG Kcal/mol value with lupeol. The ΔG Kcal/mol value was about -7.77. With Swissdock molecular docking system, the result was obtained in terms of full fitness. This lesser value of ΔG indicates, the successful approach of phytochemical Bis-Desmethoxycurcumin from Turmeric(*Curcuma Longa)* as a drugagainst emerging carcinogenic pathogen *Escherichia coli*Aminopeptidase Nenzyme. Bis-Desmethoxycurcumin can be a potent phytochemical for the treatment of Urinary Tract Infections.

CONCLUSION

It was previously known that *Curcuma longa* plant has medicinal action against UTI. Mostly UTI is caused by *E. coli.*This study was carried out to provide the theoretical basis of this observation. Using Swissdock software, molecular docking operation was performed to identify the phytochemical(Desmethoxycurcumin, flavonoids, tannis, Bis-Desmethoxycurcumin, phlobatannis, and coumarin), which can have a significant interaction with the vital UTI of the microbe. It was found that Phlobatannis, Desmethoxycurcumin, coumarin, tannis and flavonoids can form strong bond with the enzyme successfully inhibiting the metabolic cycle of the microbe. Bis-Desmethoxycurcumin was found to be not much effective in deactivating the enzyme of the microbe. Terpinoids cannot deactivate the enzyme. Thus, this study could explain that the presence of Phlobatannis, Desmethoxycurcumin, Coumarin, tannis and flavonoids provided the medicinal values to *Curcuma longa* against UTI caused by*E. coli.*

This study suggest that, Bis-Demethoxycurcumin phytochemicals from Turmeric (*Curcuma longa)* can be used as a potent molecule against *Escherichia coli.* It can be used as a basic approach to design a drug against this emerging infectious pathogen. Further in- vitro and in-vivo studies is required for the extension studies of this approach. Use of bioinformatics tool and computational biology for the drug design is a better approach to limit the time and cost that is required for the in-vitro and in-vivo drug designing studies.

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The kind support of senior management team, VC madam, Dean Sir, HoD madam, My guide and other staff members of Centurion University of Technology and Management, Odisha is highly acknowledged.

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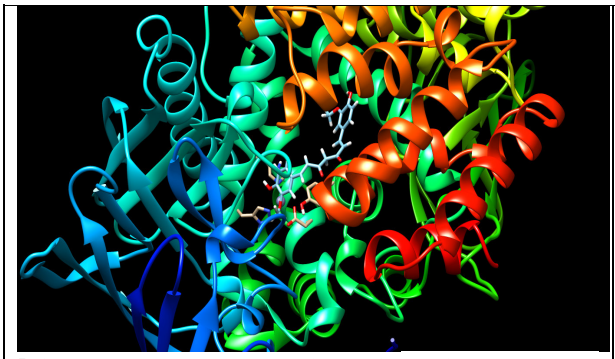
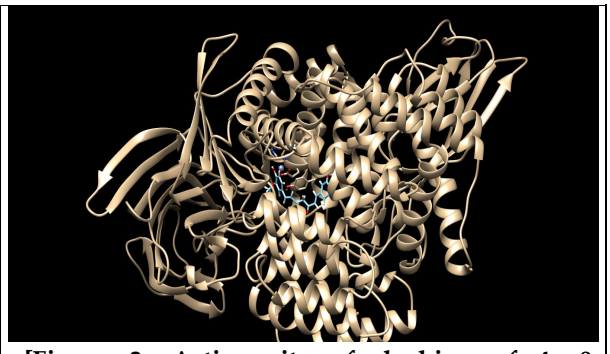


[Figure 1- PDB ID-4xn9 (ProteinAminopeptidase Nfrom *E. coli*)]



[Figure 2- Active site of docking of 4xn9 Aminopeptidase Nof *E. coli*with Swissdock viewed in UCSF chimera]

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RESEARCH ARTICLE

Computer-Aided Investigation of Phytochemicals from Tulsi *(Ocimum sanctum)* against *Streptococcus pyogenes* based on Molecular Docking Studies

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ABSTRACT

Streptococcus pyogenes (Group A Streptococcus or GAS) are widely prevalent bacterial pathogens worldwide. Human is the most common primary host of this pathogen. It causes wide range of diseases ranging from pharyngotonsillitis to potentially lethal invasive diseases such as necrotizing fasciitis and streptococcal toxic shock syndrome. Hence, development of new drugs against this pathogen is highly concern. Inosine Monophosphate Dehydrogenase (IMDH) is a key enzyme of *Streptococcus pyogenes* which catalyzes the conversion of inosine 5'-phosphate (IMP) to xanthosine 5'-phosphate (XMP), the first committed and rate-limiting step in the de novo synthesis of guanine nucleotides, and therefore plays an important role in the regulation of cell growth. So, IMDH may be a potential target for dug designing and vaccine development. In this study, we retrieved *S. pyogenes* structure from PDB and used it as a drug target protein. Phytochemicals have been used as drugs since ancestral time period. One of the potent phytochemicals of Tulsi (*Ocimum sanctum)* is Luteolin. Structure of the luteolin was retrieved from Pubchem and docking was performed by using Swissdock softwares. Swissdock is a web server specially designed to carrying out protein-ligand docking simulations. In our docking study, we found phytochemical luteolin of Tulsi is effective against Inosine Monophosphate Dehydrogenase enzyme of *S. pyogenes*. We also concluded that, in silico docking study is also a better approach to check the utility of any phytochemical as a drug than in –vivo and in-vitro study.

Key words: Phytochemical, Swissdock, Tulsi (*Ocimum sanctum*), *Streptococcus pyogenes*, luteolin, Inosine Monophosphate Dehydrogenase (IMDH)

INTRODUCTION

Streptococcus pyogenes is a major human-specific bacterial pathogen that causes various diseases ranging from mild localized infections to life-threatening invasive infections. *S. pyogenes* infection can result acute rheumatic fever, pharyngotonsillitis, necrotizing fasciitis and streptococcal toxic shock syndrome [1]. *S. pyogenes* is a gram-positive, facultative anaerobe, catalase-negative, oxidase negative, β-hemolytic streptococci. It grows best in 5 to 10% carbon dioxide, and forms distinct colonies on blood agar plates. Lancefield serological grouping system is used to differentiate group A streptococci (GAS) from other streptococci. The type A antigen of *S. pyogenes* is a polysaccharide which comprised of N-acetylglucosamine attached to a rhamnose polymer backbone [2]. M protein is the major surface protein presents on S. pyogenes cell wall. The class I S. pyogenes causes rheumatic fever and class II S. pyogenes causes glomerulonephritis. The mortality and morbidity rate due to Rheumatic Heart Disease (RHD) is high. Transmissions of *Streptococcus pyogenes* can occur through airborne droplets, hand contact with nasal discharge, surfaces contaminated with bacteria and skin contact with contaminated lesions etc [3]. The sign and symptoms of streptococcal infection includes Sore throat, fever, malaise, pharyngeal exudate, tender cervical lymphadenopathy and enlarged tonsils. The most effective treatment of streptococcal pharyngitis is oral penicillin which is a cost effective treatment also. Macrolides and first-generation cephalosporin can also be used as an alternative drug for treatment [4]. Inosine Monophosphate Dehydrogenase (IMDH) is a key enzyme of *Streptococcus pyogenes* (EC1.1.1.205) which catalyzes the conversion of inosine 5'-phosphate (IMP) to xanthosine 5'-phosphate (XMP), the first committed and rate-limiting step in the de novo synthesis of guanine nucleotides, and therefore plays an important role in the regulation of cell growth [5].

Tulsi (*Ocimum sanctum)* which is also known as holy basil is one of the extensively used medicinal plants in Ayurveda. It is having antioxidant, immune-modulatory, antipyretic, anticancer, chemo-preventive, radio-protective, anti-hypertensive and cardio protective and antimicrobial activity. Due to its widely known therapeutic value, it is most popular home remedy for Swasa (Asthma) and Kasa (Cough) in India [6]. Following is the taxonomical classification of Tulsi (*Ocimum sanctum).*

Taxonomy

Kingdom	:	Plantae
Class	:	Magnoliopsida
Order	:	Lamiales
Family	:	Lamiaceae
Genus	:	Ocimum

Preclinical studies have shown that, the most common active phytochemical of Tulsi includes eugenol, rosmarinic acid, apigenin, myretenal, luteolin, β-sitosterol, and carnosic acid etc [7, 8].

In this present study, molecular docking was performed by using Swissdock softwares. Docking is a method which predicts the preferred orientation of one molecule to a second when bound to each other to form a stable complex. Knowledge of the preferred orientation in turn may be used to predict the strength of association or binding affinity between two molecules. Docking is frequently used to predict the binding orientation of small molecule (ligand) drug candidates to their protein targets in order to in turn predict the affinity and activity of the small molecule [9, 10].

MATERIAL AND METHODS

Protein structure (PDB ID-1zfj) files of *Streptococcus pyogenes* Inosine Monophosphate Dehydrogenase (IMDH) was retrieved from PDB site containing resolution about 1.90A^0 and used as a drug target protein. Phytochemicals of Tulsi (*Ocimum sanctum)* luteolin structure was also retrieved from Pubchem. Docking study was performed by using Swissdock softwares. The value was obtained in terms ΔG Kcal/mol. Energy value is inversely proportional to the

affinity of the molecule to be used as a drug. So, lesser the (ΔG) of phytochemical molecule indicates higher affinity of that phytochemical as a drug. In online swissdock software, protein IMDH was browsed in it. The selected molecule (luteolin phytochemical) was docked at different sites of target IMDH protein. After completion of docking, the result was obtained at provided email ID. The result was analyzed at the link provided in the email. UCSF chimera was used to find the predicted binding modes.

RESULTS AND DISCUSSION

From this Swissdock molecular docking studies, we found good ΔG Kcal/mol value with luteolin. The ΔG Kcal/mol value was about -5.87. With Swissdock molecular docking system, the result was obtained in terms of full fitness. This lesser value of ΔG indicates the successful approach of phytochemical luteolin from Tulsi (*Ocimum sanctum)* as a drug against emerging carcinogenic pathogen *S.pyogenes* Inosine Monophosphate Dehydrogenase (IMDH) enzyme. Luteolin can be a potent phytochemical for the treatment of pharyngotonsillitis, necrotizing fasciitis, streptococcal toxic shock syndrome and Rheumatic Heart Disease (RHD).

CONCLUSION

This study suggest that, luteolin, phytochemicals from Tulsi (*Ocimum sanctum)* can be used as a potent molecule against *Streptococcus pyogenes.* It can be used as a basic approach to design a drug against this emerging carcinogenic pathogen. Further in- vitro and in-vivo studies is required for the extension studies of this approach. Use of bioinformatics tool and computational biology for the drug design is a better approach to limit the time and cost that is required for the in-vitro and in-vivo drug designing studies.

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The kind support of senior management team, VC madam, Dean Sir, HoD madam and other staff members of Centurion University of Technology and Management, Odisha is highly acknowledged.

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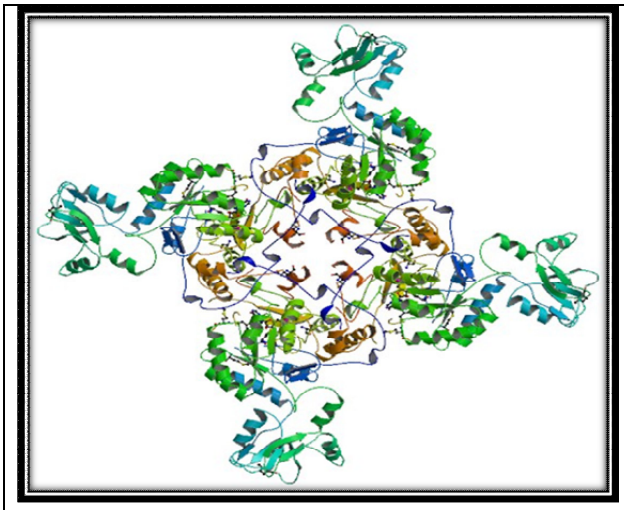

Figure 1- PDB ID-1zfj (Protein Inosine Monophosphate Dehydrogenase of *S.pyogenes*)

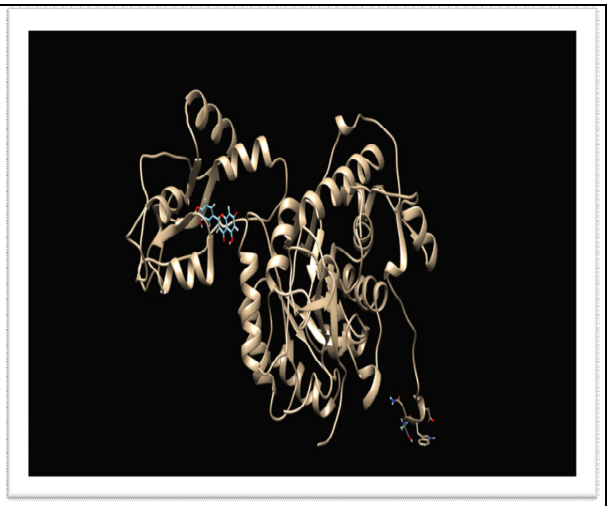

Figure 2- Docking of 1zfj (IMDH) of *S. pyogenes* with Swissdock viewed in UCSF chimera

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REVIEW ARTICLE

Dark Energy Cosmological Model and Overview

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ABSTRACT

In the present review, Demonstration was done in case of modified gravity and generalised dark energy in a way that leads to the observed accelerated expansion. By adding a non-linear term to the lagrangian of the electromagnetic field generated a fluid with a super negative and time dependent equation of state. In case of the interaction of pressure less matter and dark energy; super accelerated expansions can be obtained. Correction to the apparent horizon entropy may force the universe to tend to a de sitter space time by obtaining ultimate value of Hubble parameter and dark energy density. Generalized chaplygin gas contains some of the key ingredients in the description of the universe dynamics.

Key words: Hubble parameters, density, dark energy and dark matter.

INTRODUCTION

The universe is presently undergoing an accelerated expansion. The main agent behind it is usually called 'Dark Energy'. Dark energy is an unknown form of energy that affects the universe on the largest scales. The negative bulk pressure is the main reason behind the dark energy to cause accelerated expansion. The coincidence problem arisen is the matter of worry and in every interpretation; our first aim is to alleviate it. In this review it is clear that by choosing appropriate candidate or model (such as HDE and time varying DE) the coincidence problem is removed successfully by obtaining an accelerated universe.

Dark energy cosmological model

CDM model does not imply the physical existence of dark energy. By dropping the assumption of CDM is a perfect fluid, the data can be fitted without dark energy. In case of imperfect CDM, negative bulk pressure might be the reason behind cosmic acceleration. We think that the two phenomena- accelerated expansion and structure formation in a large scale are linked. During the formation of in-homogeneities due to dissipative processes the

effective forces give rise to accelerated expansion of CDM universe.The assumption that CDM is a perfect fluid must be tested and the discrepancy may be resolved by taking into account the gravitating mass density.

In this work a Holographic Dark Energy Model was explored in a flat FLRW Universe, which contains cold dark matter and dark energy, baryons, radiations within the frame work of General Relativity. Three types of phenomenological interactions in the dark sector were considered. The algebraic expressions for the cosmological parameters such as the deceleration and coincidence parameters were obtained. Lastly, this model was compared graphically with the □CDM model.

To describe the accelerated expansion of the Universe in the present era, sources of matter (commonly dubbed to be dark energy), which are capable of generating this acceleration are considered. A cosmological constant □ is an important candidate for dark energy, which provides a good explanation for the current acceleration. But some problem arises such as, mismatch between the expected value of the vacuum energy density and the energy density of the cosmological constant and secondly the reason behind the same order of densities of dark energy and dark matter. As an alternative, dynamical dark energy models are proposed and analysed. Among them, Holographic Dark Energy Models, originated from the Holographic Principle, plays a vital role. By taking the current components of the Universe such as baryons, radiation, cold dark matter and Holographic dark energy; a theoretical model was developed; with interaction in the dark sector. The HDE model was compared graphically with □CDM, using the referential values for the HDE parameters and the given interactions. Using Bayesian statistics with the observational data (SNe Ia, CC, BAO, CMB) the present scenarios were expected to contrast in the near future.

Constraints on the interacting Holographic Dark Energy Model:- The interacting holographic dark energy model with spatial curvature was examined here. With requirement that the Universe is experiencing an accelerated expansion using the "near flatness" condition, they had constrained the parameter space of the model. The result found from this model can explain that the model can accommodate a transition of the dark energy from $\omega_D>-1$ to $\omega_D<-1$.

Various observational data indicates that our universe is undergoing an accelerated expansion driven by a yet unknown dark energy. The leading interpretation of such a Dark energy is a cosmological constant. But recent analysis of type Ia supernova data indicates that the time varying DE gives a better fit than a cosmological constant. Theoretical attempts towards understanding of the ω_D crossing -1 phenomenon have taken place. Investigation of the interaction between DE and DM in the holographic DE model has been done by using the future event horizon as an IR cut off which explain the early deceleration and late time acceleration of our universe.

Here they have obtained the parameter space of the coupling between DE and DM and the constant c from holography. To accommodate the transition of DE from $\omega_D>-1$ to $\omega_D<-1$, they have further constrained the parameter space on b^2 and c. Lastly they have obtained the results in a closed universe.

Poly-tropic dark matter flows illuminate dark energy and accelerated expansion

Poly-tropic processes in a DM fluid have been most successfully used in modelling dark galactic haloes which improves the velocity dispersion profiles of galaxies. Here the time evolution and the dynamical characteristics of a spatially flat cosmological model was explored. In this model the DM possesses some sort of fluid like properties i.e. the fundamental units of the Universe matter-energy content are the volume elements of a DM fluid, performing poly-tropic flows. As a source of the universal gravitational field, the energy of this fluid's internal motions are taken into account. The extra energy needed to compromise spatial flatness is compensated through this energy. This model depends on only one free parameter, the corresponding (poly-tropic) exponent, Γ. In this model, for $\Gamma\leq0.541$ without DE and cosmological constant, the conventional pressure becomes negative enough so that the Universe accelerates its expansion at cosmological red-shifts below a transition value. Finally this model interprets why and when the Universe transits from deceleration to acceleration. It reveals the catalytic role of the internal motions for the onset of acceleration.

Holographic dark energy and cosmic coincidence

A wide range of discussions are carried out to know the beginning of accelerated expansion, whether it is a transient episode or last forever, what is the agent behind it etc. The agent is usually called dark energy, which must possess a negative pressure high enough to violate the strong energy condition. There are a number of dark energy candidates such as cosmological constant and a variety of exotic field (scalar, tachyon, k-essence etc). Whatever may be the candidate it suffers the coincidence problem i.e. why are the matter and dark energy densities of precisely the same order? Now a new dark energy candidate based on the holographic principle was proposed. Earlier the shortcut to quantum gravity and it's application in cosmology and black hole growth was proposed. According to this principle, the number of degrees of freedom of physical systems scales with their bounding area rather than with their volume. Then a suggestion was given that dark energy should obey this principle and DE was constrained by the IR cut off. In line with this suggestion Hsu Li argued about dark energy density which leads to wrong equation of state but his 3rd choice, the identification of L with the radius of the future event horizon gives the desired result, namely a sufficiently negative equation of state to obtain an accelerated universe.

In this letter, they demonstrate that any interaction of pressure-less dark matter with holographic dark energy, whose IR cut off is set by the Hubble scale, implies a constant ratio of the energy densities of both components thus solving the coincidence problem. The equation of state parameter is obtained as a function of the interaction strength. For a variable degree of saturation of the holographic bound the energy density ratio becomes time dependent which is compatible with a transition from decelerated to accelerated expansion.

In the paper Dark Energy versus Modified Gravity There is now strong observational evidence that the expansion of the universe is accelerating. The cause behind this accelerated expansion is supposed to be an unknown " dark energy" component. To overcome the theoretical problems arisen, General relativity has to be modified in a way that leads to the observed accelerated expansion. Here they show by demonstrating explicitly that a generalised dark energy model can match the growth rate of the DGP model and reproduce the 3+1 dimensional metric perturbations.

In this letter they have shown that the growth factor is not sufficient to distinguish between modified gravity and generalised dark energy, even if the expansion history (and so the effective equation of state of the dark energy) has been fixed by observations. They have also demonstrated that in some cases (DGP) the dark energy can match the metric perturbations completely. If the expansion history and the growth of matter perturbations were to match those predicted from a physically motivated and self consistent modified gravity model, a statistical analysis would rule out a fine tuned dark energy model. In the paper, Non-linear electrodynamics and the acceleration of the universe it is shown that the addition of a non-linear term to the lagrangian of the electro-magnetic field generated a fluid with a super negative equation of state, causing an accelerated expansion of the universe. Some general properties of non-linear electro-magnetism is cosmology are also discussed.

Here they proposed a model which displays a time-dependent EOS, with a super-negative EOS parameter as a limit. Instead of using a negative kinetic energy term for a scalar field, they modified the action for the electro-magnetic field by the addition of a non-linear term which follows Gauge invariance. This modification is harmless in case of a point charge. The result of this modification in FRW cosmology is to accelerate the universe, ending in a Big Rip. More experiments are undergoing to reconstruct the EOS from observation. This reconstruction implies the measurement of the jerk (3rd derivative of the scale factor). The model they have analysed yields an EOS with a value [$\omega_{(-1)}$=-7/3]which is disfavoured by observation. In the paper Dual interacting cosmologies and late accelerated expansion they have shown that by considering a universe dominated by two interacting components a super accelerated expansion can be obtained from a decelerated one by applying a dual transformation that leaves the Einstein's Field equations invariant. They have considered a homogeneous, isotropic and spatially flat universe dominated by two fluids (pressure less matter and dark energy) that do not conserve separately but interact with each other. In this case there is a dual symmetry transformation that preserves the form of Einstein's equations irrespective of whether the dark energy is phantom or not. Super accelerated expansions can be obtained from decelerated one with out affecting the field equations also in the case that matter and dark energy interact. If the interaction term is $\Pi=-c^2(\varrho_1+\varrho_2)$ then the cosmic coincidence problem is alleviated in the sense that there is an

attractor such that the energy densities of matter and dark energy tend asymptotically to a fixed ratio neglecting the dark energy component to be phantom or not. The input parameter cannot be derived at present. In the paper Cosmic accelerated expansion and the entropy-corrected holographic dark energy they have studied the behavior of Hubble parameter in the holographic dark energy model by considering the logarithmic correction to the energy density.

They have considered a spatially flat FRW universe dominated by ECHDE and a barotopic matter interacting through a general source term. They have taken the apparent horizon as the IR cut off. Considering the effects of thermal fluctuations around equilibrium quantum fluctuations or charge and mass fluctuations, modifies the entropy attributed to the horizon. Applying these corrections to the apparent horizon entropy they obtained an autonomous differential equation for the Hubble parameter. After obtaining the critical points they have classified the behaviour of the system in terms of the parameters of the interaction and ECDHE. For this purpose they have used algebraic features of the autonomous differential equation and LambertW functions. They obtained that the correction terms may force the universe to tend to a de sitter space-time at late time. Also obtained the possible ultimate value of the Hubble parameter and also derived the corresponding dark energy density. The coincidence problem is also alleviated. In addition they have studied some necessary conditions for the model to describe the acceleration phase in inflation era. The inflation was assumed to be transient and the possible values of the Hubble parameter at the end of inflation were derived.

In the paper Generalized Chaplygin Gas, Accelerated Expansion and Dark Energy-Matter Unification they have considered the scenario emerging from the dynamics of a generalized d-brane in a (d+1, 1) space time. The generalization of the chaplygin EOS describing this system is given in terms of the energy density ϱ and pressure p by the relation $p = - A/\varrho^{\alpha}$, where A is a positive constant and $0<\alpha\leq1$. As in the case of the chaplygin gas (for $\alpha=1$) this model admits a d-brane connection as its Lagrangian density corresponds to the Born Infeld action plus some soft logarithmic corrections. Here the space time is shown to evolve from a phase that is initially dominated, in the absence of other degrees of freedom on the brane, by non-relativistic matter to a phase that is asymptotically De Sitter. This behaviour is similar to one of the Chaplygin gas. The intermediate regime in this model corresponds to a phase where the effective EOS is given by $p=\alpha\varrho$. They have estimated the fate of the in-homogeneities admitted in the model and shown that these evolve consistently with the observations as the density contrast they introduce is smaller than the one typical of CDM scenarios and closer to the ones predicted by the □CDM in comparison to the Chaplygin $\alpha=1$ case. Hence, the Chaplygin gas contains some of the key ingredients in the description of the Universe dynamics at early as well as late times.

CONCLUSION

Various observational data indicates that our universe is undergoing an accelerated expansion. A wide range of discussions are carried out to know the beginning of accelerated expansion; whether it is a transient episode or last forever; what is the agent behind it?. The agent is usually called 'Dark Energy' which must possess a negative bulk pressure high enough to violate the strong energy condition. There are a number of dark energy candidates such as □-cosmological constant and a variety of exotic field (scalar, tachyon, k-essence etc). Whatever may be the candidate it suffers the coincidence problem i.e. why the matter and dark energy densities are of precisely the same order? To overcome the coincidence problem or to alleviate it more suitable alternatives to cosmological constants were chosen such as time varying Dark Energy, Holographic dark energy etc. To overcome the theoretical problems, different models (CDM, □CDM, HDEM etc.) were considered and observations were taken. The results found were in-terms compared with the pre-existing ones. The different models and their results may be summarized as: A spatially flat cosmological model depending upon only one free parameter, poly-tropic exponent Γ was considered; where for $\Gamma\leq0.541$ without DE and cosmological constant, the conventional pressure becomes negative enough so that the universe accelerates its expansion at cosmological red shifts below a transition values.

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RESEARCH ARTICLE

Evaluation of Relaxation Time, Acoustic Impedance and Gibb's Free Energy of Edible Oils through Ultrasonic Technique

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ABSTRACT

In the present work,Density, Viscosity and ultrasonic velocity at a frequency of 4 MHz and in the temperature range 303–318 K are measured in some of the edible oils, namely Palmolein oil,Groundnut oil,Mustard oil,Sunflower oil.Various physical parameters such as relaxation time, acoustic impedance and Gibb's free energy of have been estimated using measured data on velocity viscosity and density. These values of relaxation time, acoustic impedance and Gibb's free energy and their variations with temperature in the systems of oils studied.Theultrasonic technique become very important to characterize the oils and fats.It is used as a versatile tool in study of internal structure and inherent properties of fats and oils, since it does not change the properties of the structure of materials.The variation of rheological and ultrasonic parameters in the oils are studied and reported in present paper.

Key words : Acoustical parameters, density, edibleoils and ultrasonic velocity.

INTRODUCTION

Ultrasonic liquids studies are of great use in understanding the nature and strength of the oil molecular interactions [1].This research is focused on illustrating the utility of the ultrasonic technique in composing different forms of edible oil. Theease, functionality and low cost of ultrasonic methods used to analyze them as vital components in laboratories of research.The edible oils contain both fatty acids and triglyceridesin their composition [2-4].Fatty acids are straight chain aliphatic compounds terminated with a group–CCOHand triglycerides arepropane esters 1, 2, 3-triol with threere sidues of fatty acid(fig 1 and fig2). Auto-oxidation produced during the storage and heatingis well known to be considered a primary cause of edible oil erosion [5]. The goal of the present work is to analyze some widely used edible oils experimentally,using an ultrasonic approach to gain an useful information into their dynamic properties.The relaxation time, acoustic impedance and Gibb's free energy are closely related to the physico-chemical

properties of the oils by which sound waves travel and can thus be focused on providing evidence on all these properties [6-7].

MATERIALS AND METHODS

Different standard edible oil like mustard, groundnut, palmolein & sunflower were collected from business units as samples to compare & investigate different characteristics & dynamic properties.

Due to their common market availability, the different types of edible oil, which are palmolein oil,groundnut oil,mustard oil,sunflower oil was chosen. It proves that consumer are interested in buying this type of edible oil on their daily basis as opposed to any other vegetables oil that is difficult to obtain from oils that are identified as vital nutrients for consumers. They provide the most focused energy source of any foodstuff, supply essential fatty acids and contribute significantly to the pleasure of cooking. The findings of this analysis showed the different types of edible oil are analyzed in four different regulated temperatures to determine the impact of temperature on the ultrasonic velocity values. Methods adopted are equivalent to in my earlier paper [8]

THEORETICAL ASPECT

The information of ultrasonic speed, ϱ, and η lead to the determination of different thermo-acoustical parameters, using standard equation.

Relaxation time $\tau = \frac{4}{3}.(\beta.$

Acoustic impedance $Z = \rho.U$

Gibb's free energy $\Delta G = 2.30.KT\log\left(\frac{KT\tau}{h}\right)$

Where, 'τ'is the relaxation time, Adiabatic compressibility 'β' 'T' is the absolute temperature, 'K' is the Boltzmann's constant and 'h' is the Planck's constant.

RESULTS AND DISCUSSIONS

The density(ϱ),viscosity(η) and velocity(U) of oil samples are reported in my earlier paper[].The Relaxation timeof oil samples is given in table 1 and variation between Relaxation timeand temperature is shown in fig.1.The Acoustic impedanceof oil samples is given in table 2 and variation between Acoustic impedanceand temperature is shown in fig.2. The Gibb's free energy of oil samples is given in table 3 and variation between Gibb's free energy and temperature is shown in fig.3. Relaxation time (τ) decreases slowly with increase in temperature in case of Palmolein oil and Groundnut oil, but decreases rapidly as temperature increases from 308 K for mustard oil and sunflower oil this is due to the presence of more percentage of saturated fatty acids in both Palmolein oil and Groundnut oil. With increase in temperature the presence of unsaturated percentage of fatty acids leads to decrease of relaxation time for Sunflower oil and mustard oil. The former indicates lack of strong molecular interaction between the components of the oils, and the latter is true because of instantaneous conversion of excitation energy to translational energy.

In the present system the values of acoustic impedance are less in Palmolein oil as the percentage of saturated and un saturated fatty acids are nearly equal and is more in the case of mustard oil and groundnut oil due to the more number of double bond. Where as in case of Sunflower oil more percentage of un-saturated fatty which is decreases the acoustic impedance rapidly by increasing the temperature which leads to less intermolecular interaction among the molecules. Gibbs' free energy decreases with increase in temperature of oils. Decreasing value of Gibbs function suggests that separation of like molecule is due to hydrogen bonding. The decrease in Gibb's free energy also suggests longer time for rearrangement of the molecules in the oils.Palmoleinand ground nut oil's Gibbs free energy gradually decrease at higher temperature. The Gibb's free energy for mustardoil and sunflower oil decreases at

higher temperature. It is due to depends on the percentage of saturated fatty acids and un- saturated fatty acids contained by the oils.

CONCLUSION

The report clearly shows that the ultrasonic parameters focus on the percentage of un-saturated fatty acids and saturated fatty acids that the different edible oil comprise. Edible oils are described in terms of their fatty acids,and its flow activity with temperature could be well characterized by ultrasonic technique. The chemical changes are related to the ultrasonic changes parameters such as relaxation time, acoustic impedance and Gibb's free energy may be used to define adulteration,track the consistency of the oil and thermal degradation in oils.

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Figure 1

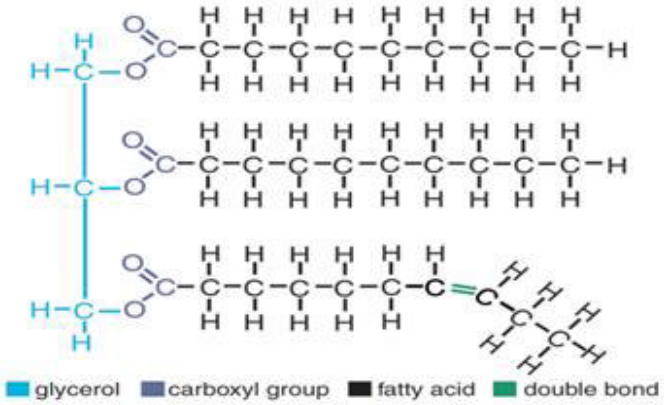

Figure 2

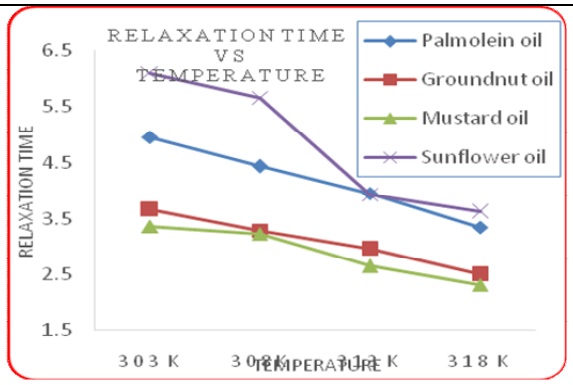

Fig.3 Variation of Relaxation timeof oils with different temperatures

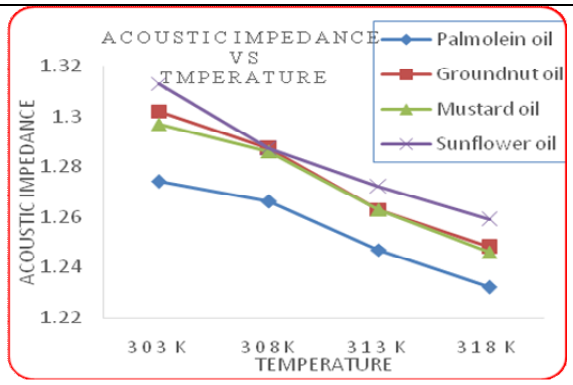

Fig.4 Variation of Acoustic impedance of oils with temperatures

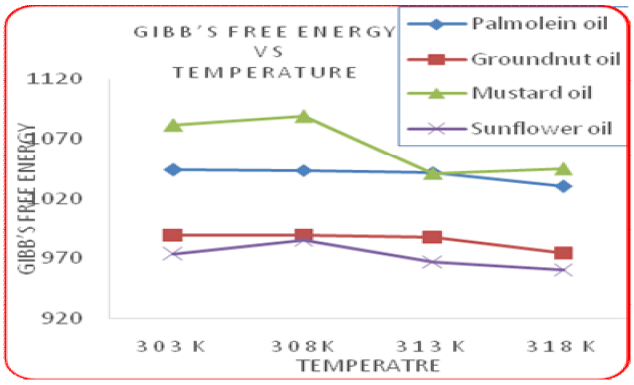

Fig. 5 Variation of Gibb's free energyof oils with temperatures

Table-1 Values of Relaxation time (τ) of different oils

T (kelvien)	Relaxation time (τ)(10^{-15} S)			
	Palmolein oil	Groundnut oil	Mustard oil	Sunflower oil
303 K	4.953	3.662	3.364	6.081
308K	4.435	3.294	3.231	5.656
313 K	3.953	2.955	2.651	3.937
318 K	3.349	2.503	2.328	3.618

Table-2 Values Acoustic impedance (Z) of different Oils

T (kelvien)	Acoustic impedance (Z):- Z = U.ϱ(×10^6 kg·m^2·s^{-1})			
	Palmolein oil	Groundnut oil	Mustard oil	Sunflower oil
303 K	1.274	1.302	1.297	1.313
308K	1.266	1.287	1.286	1.287
313 K	1.247	1.263	1.263	1.272
318 K	1.232	1.248	1.246	1.259

Table-3 Gibb's free energy (ΔG) of different oils

T (kelvien)	Gibb's free energy:-ΔG = $K_B T.Ln (K_B T\tau/h) 10^{-23}$			
	Palmolein oil	**Groundnut oil**	**Mustard oil**	**Sunflower oil**
303 K	1043.8	988.9	1081.1	973.5
308K	1043.7	988.7	1088.6	985.1
313 K	1042	987.4	1041.3	967.1
318 K	1030.1	974.5	1044.8	960.7

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RESEARCH ARTICLE

Healthcare Awareness; She Decides on Her Health, Her Future

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ABSTRACT

Women must be aware about the health hazards and its impact in their life, including their own lifestyle and food habits – not least because it can lead to other life-changing decisions. If an adolescent girl does not get this education at her early age, it can lead to multiple complication in post marriage life. With enough awareness a girl can lead healthy life and a family too. For example, If a woman maintain minimum gap between giving birth to 2nd child, she can get enough nutritious food and take care herself and her children. Similarly,if an adolescent girl takes HPV vaccine, can reduce her chances of getting cervical cancer, averting illness and potentially catastrophic health expenditures in the future. The common health problems like; PCOS, HYPOTHYROIDISM, ALOPECIA AND MATERNITY are the great concern for girls at their adult stage.The research was made to know the awareness level on health issues and it'spreventive measures among the rural girls followed by a health awareness programme for healthy life.

Key words: Healthcare, HPV Vaccine, PCOS, Hypothyroidism, Alopecia and Maternity

INTRODUCTION

Adolescence is a beautiful length of life and generally a healthful one. Childhood illnesses are left at the back of and with a little care one can build up a lifetime of properly health. But this is additionally a duration when a individual is most vulnerable; the standard growth and improvement and additionally the physical, reproductive and psychological modifications expose the teenagers to many health risks. Careful and unobtrusive attention to every thing of fitness at this stage will assist will assist young people develop into wholesome and responsible adults. One of the most common heath concerns amongst adolescent ladies in our us is undernutrition and anemia. One third of the adolescent women in India are underweight and as per the NFHS three data, fiftysix p.c are anemic. Poor nutrition, worm infestations and menstrual abnormalities, both menorrhagia and,polymenorrhea make a contribution to this without problems preventable condition. Many of these girls are born with deficient iron stores due to the fact their moms were anemic in the course of pregnancy.

Poorcognitive functions and widespread ill health affect their conceivable to attain the best in studies and other activi ties. Although iron supplementation is recommended for adolescent girls, it is healthier to enhance their standard eating regimen as these women have diets deficient in calories, proteins and other crucial nutrients. Good food plan is quint essential for applicable boom and improvement of adolescents, for boosting their immunity and stopping conditions like anemia. Vitamin D and calcium in weight-reduction plan and weight bearing workouts construct up the bone mass in this age. Peak bone mass is achieved via about 30 years of age and begins declining thereafter. A low peak bone mass is an vital threat issue for osteoporosis later. Malnourishment and weight problems regularly seen in prosperous teenagers can additionally predispose them to fitness problems like polycystic ovary and metabolic syndrome. Emphasizing the importance of a well balanced healthy weight-reduction plan and enough physical endeavor at this age can go a lengthy way in ensuring properly health later.

Reproductive fitness issues of adolescent girls additionally need to be addressed. Many myths encompass the regular menstruation. Educating them about this physiological situationallows them to cope up with many of the troubles and lets in them normal things to do with no restrictions in the course of menstruation. Irregular and infreq ent cycles are frequently viewed for a few years after menarche and don't want any intervention. Irregular cycles with obesity, hirsutism may be due to polycystic ovarian sickness but need to be investigated to rule out different reasons of hyperandrogenism like congenital adrenal hyperplasia or ovarian tumor. Heavy menstrual bleeding requires complete comparison such as hemoglobin estimation and coagulation profile as some congenital coagulation issues may appear as puberty menorrhagia. Dysmenorrhea, if serve additionally wants to be investigated thugh mild dysmenorrhea can effortlessly be managed with simple analgesics. In adolescents with amenorrhea, menorrhagia or extreme dysmenorrhea, pelvic ultrasound may additionally be required to rule out any pathology. Proper and timely administration of any pathology so detected helps restoration the health of the young people.

Maintenance of right hygiene especially during menstruation is important. Poor menstrual hygiene and early sexual exposure can lead to reproductive tract infections with lengthy term morbidities. Sexually transmitted infections may additionally persist as chronic or recurrent infections and might also lead to pelvic inflammatory sickness involving cervix, uterus, fallopian tubes and ovaries. Tubal contamination can also lead to tubal bloakage and infertility later. Vaginal and cervical epithelium is immature in this age and is more inclined to infections. Human Papilloma Virus (HPV) contamination obtained at this age may later lead to premalignant or malignant adjustments in the cervix. Early unprotected sexual pastime exposes them to the hazard of HIV infection also. Teenage pregnancies may additionally adversely affect the health of the lady and can also have long time period penalties specifically if risky abortions are resorted to. Health education together with sex training must be handy to all youth whether they attend the college or not.

REVIEW OF LITERATURE

Women's fitness includes a large range of focal point areas, such as: Birth control, sexually transmitted infections (STIs), and gynecology. Breast cancer, ovarian cancer, and other lady cancers. Other ailments are like PCOS, HYPOTHYROIDISM, ALOPECIA AND MATERNITY problems. Polycystic ovary syndrome (PCOS) is a condition that influences a woman's hormone levels. Women with PCOS produce higher-than-normal quantities of male hormones. This hormone imbalance reasons them to ignore menstrual periods and makes it harder for them to get pregnant. PCOS additionally causes hair increase on the face and body, and baldness. And it can contribute to long-term fitness troubles like diabetes and coronary heart disease. Birth manage drugs and diabetes pills can help restore the hormone imbalance and enhance symptoms. PCOS is a problem with hormones that impacts female at some stage in their childbearing years (ages 15 to 44). Between 2.2 and 26.7 percent of ladies in this age group have PCOS (1, 2Trusted Source).Many ladies have PCOS but don't comprehend it. Hair loss, additionally recognised as alopecia or baldness, refers to a loss of hair from phase of the head or body. In the majority of cases, hair falls out in small patches round the dimension of a quarter. For most people, the hair loss is

nothing greater than a few patches, although in some instances it can be greater extreme. Hypothyroidism is when the thyroid gland does now not produce adequate thyroid hormones to meet the wants of the body. The thyroid is underactive. The contrary is hyperthyroidism, where the thyroid produces too a good deal thyroid hormone.

Research Objective

- Study the awareness level of girls about health issues and the it's preventive measures
- Creating awareness among girls regarding different health hazards.

Research Design

The data was collected from both primary and secondary study. It was a quantitative research with a sample size of 60. The research was done by interview methodsthrough a questionnaire. The awareness campaign was conducted to find post training response from same sample to measure their level of awareness.

RESULT ANALYSIS

The study was made to know the level awareness on preventive measure and health issues before and after the awareness programme was organised

Healthy diet and through exercise you can control PCOS

Before the training program 83% of girls had idea about this but after the training 95% of girls got the knowledge of this cure.

Acupuncture is an alternative treatment for PCOS

Only 33% of girls knew that acupuncture is an alternate for PCOS but after the program 85% of girls got the idea about it.

Rubbing green tea into your hair will help in preventing hair fall

Only 58% of girls knew that rubbing green tea is helpful for preventing hair loss but after the training 89% of girls got the knowledge.

Walk, swim or bike for 30 minutes a day helps balance hormonal levels, reducing stress levels besides reducing hair fall

Before the program only 45% of girls are aware of the fact that swim, bike or walk for 30mins for a day helps in reducing the stress level but after the programme it becomes 79%.

Only 89% of girls were knew that applying crude onion juice helps in reducing the hair loss but after the training programme 97% of girls got the idea.

Food having high selenium, zinc and vitamin-B helps in curing Thyroid

Before the programme only 89% of girls were aware of it but after the training 97% of girls got the knowledge that food with high selenium, zinc and vitamin-B helps in curing Thyroid.

Constipation and dry skin are the symptoms of Hypothyroidism

Only 49% of girls knew that the constipation and dry skin are the symptoms of Hypothyroidism but after the training programme 87% of girls got the idea.

Untreated Thyroid causes problem during pregnancy

Before the training session only 38% of girls knew about the fact that untreated Thyroid causes problem during pregnancy but after the training 91% of girls got the knowledge.

Late marriage causes pregnancy problems

58% of girls had the idea that late marriage cause pregnancy problems where as after the training session 88% of girls got the idea about it.

Abortion creates problems for conceiving in future

83% of girls already had the knowledge of abortion which creates problems for conceiving in future but after the programme 98% of girls got clear about it.

Getting pregnant in a late age increases the chances of having a baby with birth defect

Before the programme 58% of girls only knew that late age pregnancy creates the chances of having baby with a birth defect but after the programme 94% of girls got the knowledge.

CONCLUSION

The past few decades have seen impressive advances in women's health, including their sexual and reproductive health and rights. At this critical juncture, we must do all that we can to ensure that we continue to move forwards, not backwards. WHO is resolutely committed to playing its part by providing the standards and scientific evidence that underpins advances in women's and girls' health, data and estimates on the scale of the challenges, and innovative ideas on how to overcome them. Hence it is essential to have clear policy and programme designed to create awareness about health issues of girls at school level to protect them from serious complication in future and make a healthy society.

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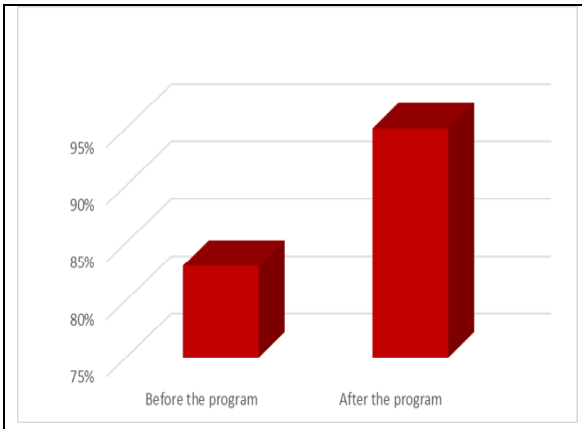
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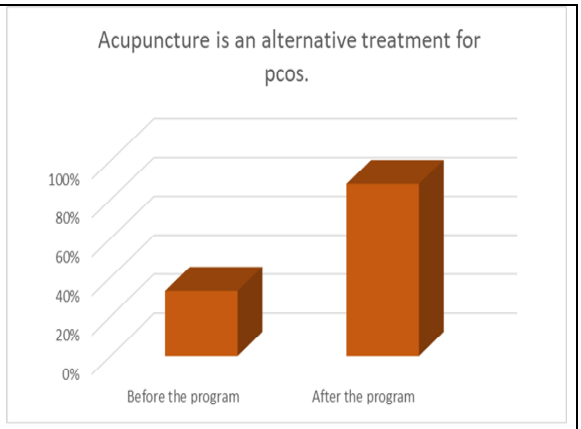
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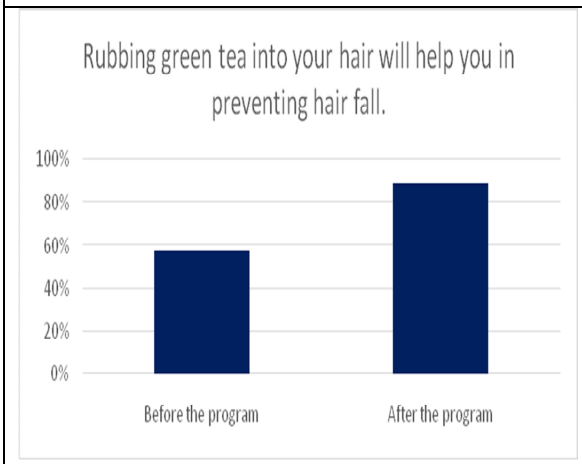
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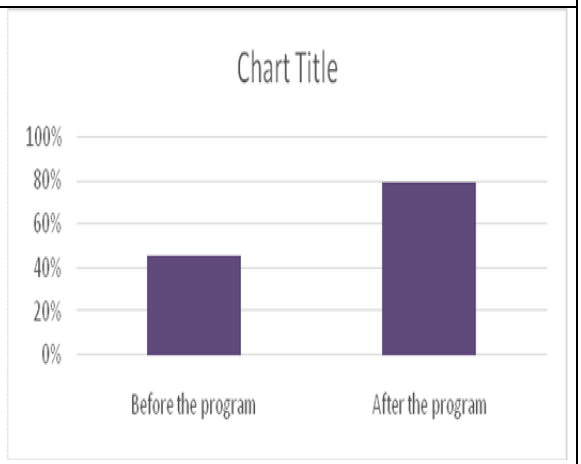
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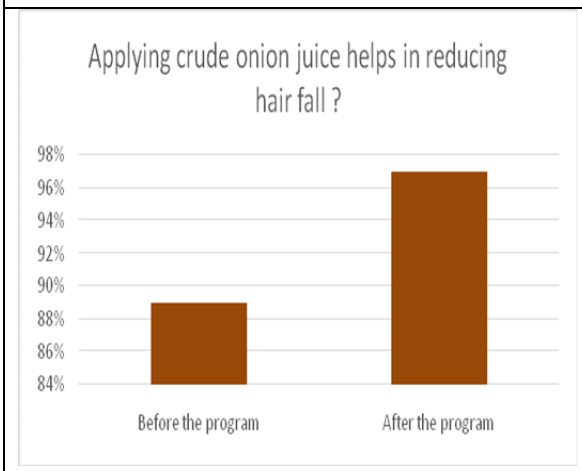
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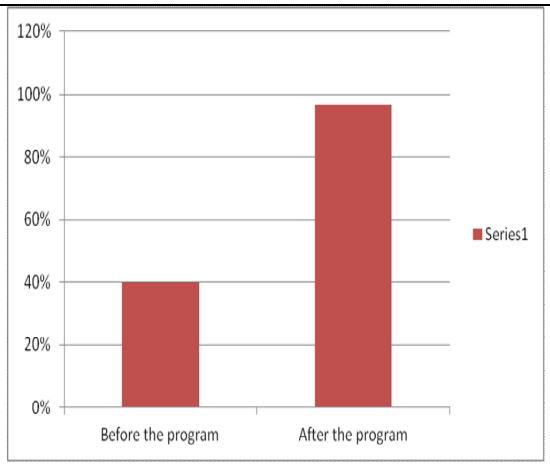
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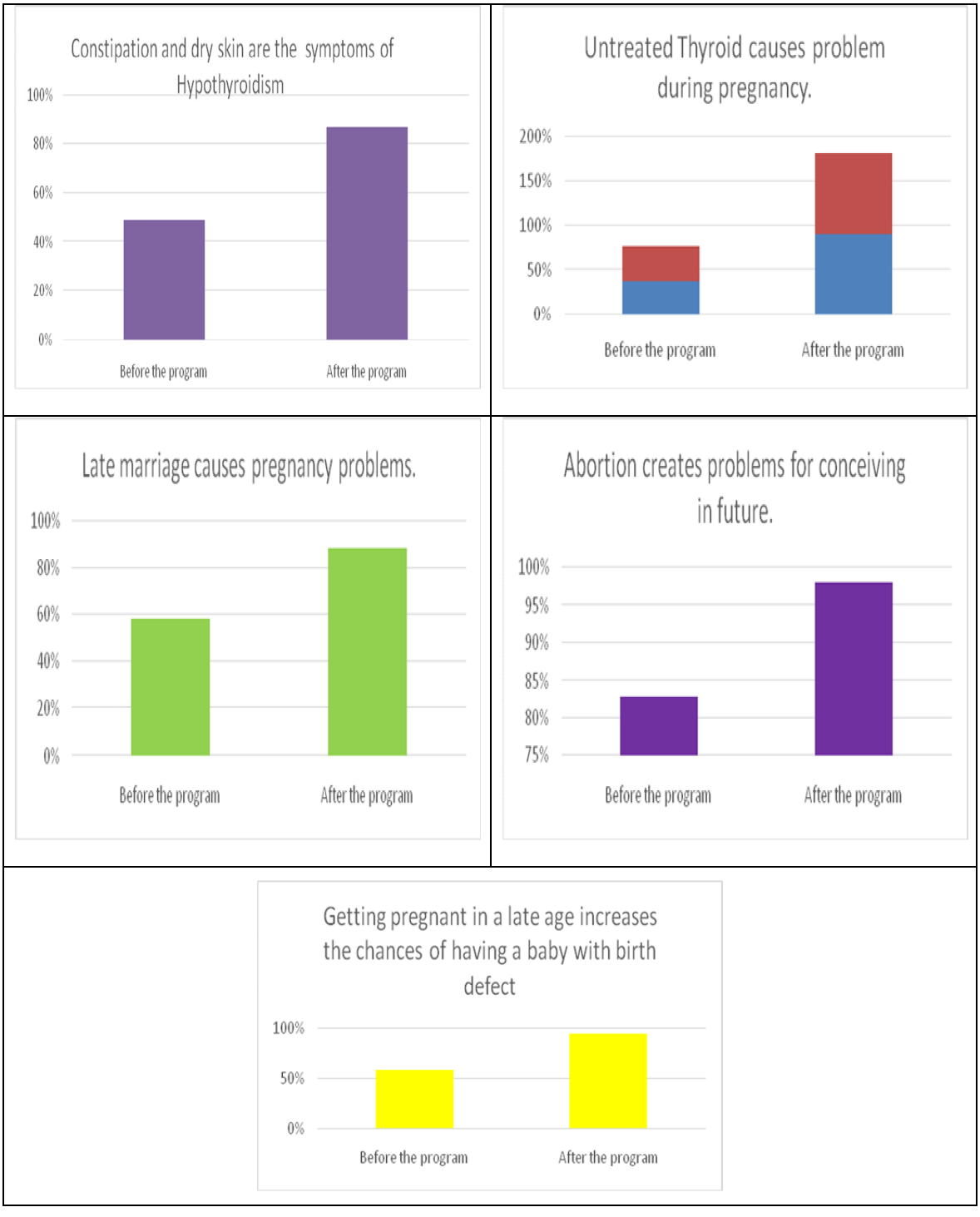
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RESEARCH ARTICLE

Skill Training in Retail and Hospitality; A Successful Model to Create Employment for Youth in Service Sector

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ABSTRACT

The value based Education, job skill and active learning are basic elementsto sustain and continue to performbya person in today context. It improves the employability conditions and the quality of life, and contribute to social and business development. Acquiring required industry Skills and upgrading with the changing environment are the basis for the competitiveness of economies and enterprises. From a social perspective, this is a tool to eradicate poverty, giving right opportunity for the marginalised under privileged youth of the society.India is fastest developing country in the world with over 50% of the population under 30 years. It is estimated, India will have the 25% of the total global workforce (World Competitiveness Yearbook, 2012)by about 2025. Hence, there is a need to have well framed policy to develop and empower the human capital and for nation's global competiveness.The research was conducted in Retail and Hospitality (R & H) training offered by GTET, one of the leading skill training centre in Bhubaneswar, Odisha, in collaboration with CCD. This skill training has created employment opportunity for young boys and girls, mobilised from rural area and then subsequently moved to work in metros of India. This training has changed their Lifestyle and also given opportunity to grow to the level of Managers in Retail and Hospitality industries. The research was made to understand the impact of skill training in creating employment opportunity for 10th/+2 pass youth with a scope to pursue graduate degree in Retail and Hospitality(BBA) while working at CCD outlet. The research aims at finding the impact of skill training in Retail and Hospitality for youth of Odisha. The study reveals that skill training has not only created employment opportunity for school dropout but also shown them a path to grow professionally in acquiring higher education while earning.

Key Words: Skill development, Retail and Hospitality, Gram Tarang, Caffey Coffey Day

INTRODUCTION

India with larger populations of youth have both positive and negative aspect in terms growth of the country. The current education systems do not facilitate to provide necessary skill and competency that can help a youth to serve in an industry or to start own enterprise. Therefore, the Govt. of India started Skill India mission to provide necessary hands-on skill for school dropout to make them industry ready. This skill training also provides ample opportunity to set up small and medium enterprise, enabling additional employment opportunity for youth. Retail and hospital Industry are key player in India today in adding value to the GDP of the country. This has also created a large employment in private sectors for school dropout up to a professionally qualified graduate.

Gram Tarang Employability Training(GTET) is the largest skill training provider in India in various fields with a strong partnership with Industry. GTET has created workshops that are well equipped with machine/equipment of industry standards and a strong curriculum recommended by industry. Retail and Hospitality is one of the most successful skill training programme offered by GTET in collaboration with Cafe Coffee. The training is offered for 3 months duration followed by 9 months on job training with stipend in any retail outlet of CCD. Since the trainees have to deal with different profile of customers, The training module has integrated a life skill training programme to take care of soft skill of all trainees along with technical training that requires for a Brew Master to make coffee and serve.After successful completion of training they get placed in retail outlet of CCD. GTET also has tie-up with Centurion University to offer BBA in Retail and Hospitality to these training post placements that create path for them to get promotion and higher growth.

The success of skill training largely depends on success story of these youth that spreads in their village, taluk and district. It helps skill training providers to mobilise these youths who normally are very reluctant to move out from their location to urban. Many such youth would be there to travel 1st time in a train to urban city and stay away from their family and relatives. Hence there is a need for training providers to make an impact assessment of skill training in achieving the very cause of Skill Indian mission and economic prosperity of unemployed youth at large.

National Skill Development Corporation Initiative in India

As per NSDC vision, the present the capacity of skill development in India is around 3.1 million persons per year. India can move to 15 million annually. Government of India has target of creating 500 million skilled workers by 2022. Thus, there is a need for increasing capacity and capability of skill development programs.The skill development initiatives will harness inclusivity and reduce the economic and social boundary such as gender, rural/urban, organized/unorganized employment and traditional/contemporary workplace.The skill development mission support the industryin creating skilled workers who are flexible to the changing demands of industry. This strategy will promote excellence and can meet the requirements of knowledge economy.

The skill development initiative not only created employable skilled worker but also shown a path to be self-employed through own start up. The skill development initiatives support employment generation, economic growth and social development processes. Skill development policy will be an integral part of comprehensive economic, labour and social policies and programmes.

Governance of skill Development Initiative

The Ministry of Skill Development and Entrepreneurship is driving skill India mission through NSDC, which has further created 38 Sector Skill Council(SSC) to develop industry specific curriculum for skill training. SSC determine skills/competency standards and qualifications and getting them notified as per NSQF. It does standardization of affiliation, accreditation, examination and certification process in accordance with NSQF as determined by NSQC. It also conducts skill-based assessment and certification for QP /NOS aligned training programmes. It funds it's training partners to run skill training programme under various schemes viz; PMKVY, DDU KY etc.

LITERATURE REVIEW

The literature review has enabled the researcher to explore wider scheme of skill training related to specific job skill. It has helped the researchers to understand the current knowledge in the field of skill training. The study highlights the impact of skill training in creating employable youth, without having formal educational degree, through research done by other researchers. It has given insights on training prospects, benefits and challenges in skilling India, skill development in creating employment and research gaps to be filled by further research

Gupta and Agarwal (2018), conducted a study on "Training Prospects in Power Sector in India". The objective of the study was to identify training need in the power sector. It also tried to find the type and level of skill trainings offered and the kind of, the organization involved in imparting such trainings. The study covers public and private players involved in imparting such training in power sector. The study found that training programs conducted for every level of jobs through various modes like short term, long term, and workshop, graduate and post-graduate programs in power sector. Theefforts are being made to re-skill the prevailing workforce and updating them with the new avenues available and approaching into the arena. Still there's a gap between the kind of skill manpower required vs. the manpower available to serve this sector. This sector can absorb large no. of skilled manpower in the field of Service, maintenance, installation, repair work and also in manufacturing. The sector skill council has already floating some skill training programme that helps in creating skilled manpower for power sector.

Shrivastav and Jatav (2017),conducted a study entitled "An Analysis of Benefits and Challenges of Skilling India" The aim of the study was to check the prospects and challenges for skilling in India. The Researcher tried to analyse the challenges and ability for creating an eco-system in terms of economic resources and sustainable knowledge has been gathered from the secondary sources for the study. The study discovered varieties of skill training offered by NSDC to generate job opportunities in line with job skill identified by industry. The study found the resource capability, the gap and initiatives taken by specific sector skill council and it's training partners. The training organisation are in need of industry standard labs/workshops to provide hands-on experience to make all trainees market ready.

It is evident that there is lot efforts are being made at various level with focused attempt and support by Govt. of India to create employable manpower to serve industry as well as to be self employed irrespective of having or not the basic formal degree. Employment generation is the one issue other than that employability and productivity is another issue. Currently about 26 million youth are getting into a age group for employment every year with about 65% of them looking for jobs. Age and formal education degree is a constraint that affecting for skills development, because of social stigma. Good news is that today, there is no bar in gender for acquiring specific skill for their employment. To make "Make in India" project successful, youth of the nation should be empowered with formal education, technical and vocational training to meet the Industrial requirement as per global standards.

Research Gap

The skill training programme has a long term social benefits in creating employment through skill training. It is essential for all stake holders to have wider prospect of knowledge and feedback on the entire training activity;

- The quality of training programme and activity undertaken in supply chain; starting from mobilisation to post placement support
- The experience and Success story of trainees,
- Trainer's experience
- Employer views.

Research Objectives

Based on need and importance of skill training in our country the researcher tries to find insights that would help all stake holders to take appropriate action as deemed fit.

- To understand the supply chain of skill training services delivered by training organisation

- To highlight experience of trainees and their success story
- To make an impact assessment of the skill training in Retail and Hospitality
- To suggest scope for improvement in training by training providers, funding agency and future participants

Research Design

The research is more qualitative and exploratory in nature.Researcher has administered a structured questionnaire to get specific data with reference to Research Objectives. The data received was compiled and presented in the form of graph/chart supported with data table.

RESEARCH METHODOLOGY

This research is explorative in nature. The researcher has studied the training Programmes and its impact on creating Employment and Self Employment of youths. The Study is in reference to Retail and Hospitality skill training only. Research methodology is divided into five sections i.e. Section I contains Data Sources, Section II analysis of data collected from trainees.

Data Sources and Data Collection

The data required for the study was collected from primary sources on multistage random sampling method from trainees through a structured questionnaire and face to face interview. The secondary sources include books, journals, handbooks, newspapers, circulars, bulletins, working papers, reports, websites and Government departments.

RESULT AND DISCUSSION

The analysis and interpretation of the various opinions given by the various respondents which were collected from the trainees are shown in the form of tables below.

Analysis and Interpretation

- The trainees were asked to respond on the reason for choosing this training programme based on specific criteria. It was found that 95% students have joined this training to get job in an industry.
- Data table; Reason for joining L&H training programme
- One of the key challenge for training organisation to mobilising youth for skill training and equally for trainees to know about such training programme and join. The trainees were asked to respond on knowing about this training.
- Data table; Reason for joining L&H training programme
- The trainees were also asked about the alternative ways to earn for their livelihood, in case non availability of such skill training
- The survey was conducted to capture the trainee experience at training organisation. It was on training and training facility available for them to rate in scale of Excellent, Good, Satisfactory and Poor.
- Data table Experience of trainees at training organisation
- The researcher tried to find more specific input on teaching input, level of skill acquired and their confidence of getting suitable employment after successful completion of this training.
- Data table; Level of industry skill acquired by trainees
- The opinion of trainees was collected on scope of improving R & H training programme and creating awareness about this for rural youth to enrolled.

SUMMARY AND CONCLUSIONS

The current study reveals that skill training in Retail and Hospitality has been a successful model to provide industry practice input, due to strong collaboration of Industry in creating training module, training materials, machine and equipment, raw materials, qualified trainer and required infrastructure. The quality of training has been endorsed by employer by giving 100% placements support. The training has made an impact in giving all round development of trainees both in technical and soft skill. The Life Skill training programme has adequately improved speaking skill in English, the art of dealing customers at retail outlet, managing the retail store. Apart from this, the trainees have the opportunity to get additional degree in BBA-Retail and Hospitality, which has made them eligible to get promotion in the organisation the level of Managers and above. It also gives a wider opportunity to serve any other Retail or Hospitality organisation. There has been few success story of trainees who have participated in various level of Brew master training and own recognition.The research was limited to trainees' experience only during training programme. The research can further be extended to take feedback from employers, parents and Alumni to have a holistic view on success of skill training in Retail and Hospitality.

Considering the need for creating employable human capital it is essential to bring a reform in formal education viz; integrating vocational courses at school level for kids to explore and many of them may not be good at studies but very good in hands-on skill. There has to be proper counselling about the career scope based on one's academic performance and passion. Similarly, it is also essential to identify skill that can be integrated at higher education level and students are given choice to pursue as elective or specialisation, which is dynamic in nature that coupled with technology and practice.

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Fig. 1 : Reason for joining L&H training programme

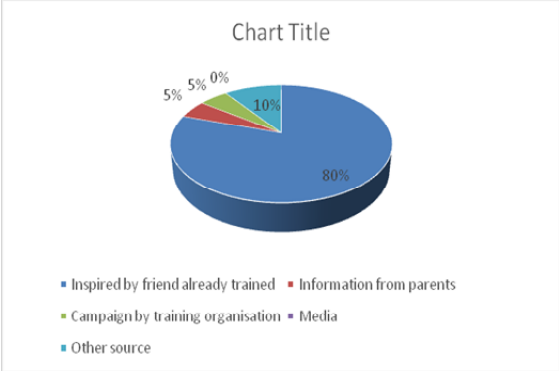

Fig.2 : Reason for joining L&H training programme

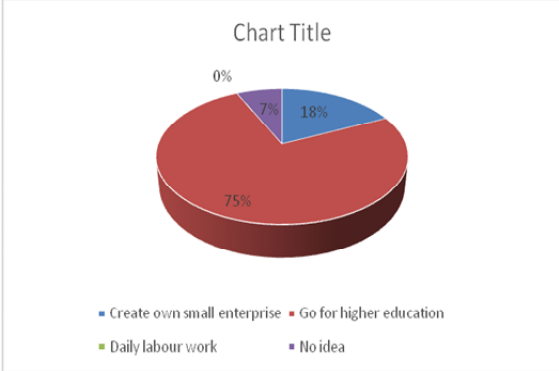

Fig.3 : Alternative option for livelihood

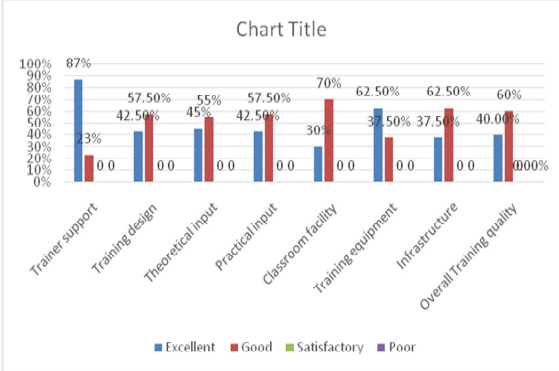

Fig.4 : Experience of trainees at training organization

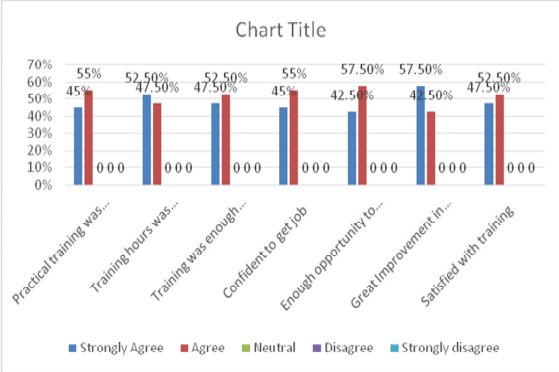

Fig. 5 : Level of industry skill acquired by trainees

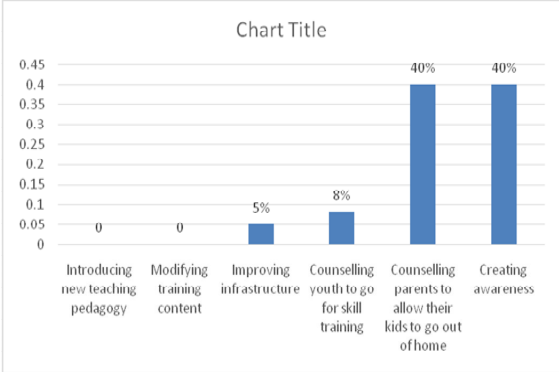

Fig.6 : Suggestion by trainees

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RESEARCH ARTICLE

Apparel Skill Training; Empowering Women Youth for a Better Life

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ABSTRACT

India is the 2nd largest population in the world with 70% of the population lives in Rural area. About 27% are from the age group of 0-14 and about 18% are from 15-24 age group. (India Demographics Profile 2019; index mundi). The youth dependency ratio is about 43.6%. The school dropout ratio is quite high in case of female child for various reason and hence they do not find suitable employment opportunity, more specifically in rural sector to earl livelihood. The skill India mission under "Apparel Made-Ups and Home Furnishing Sector Skill Council" under NSDC is doing extremely well in skilling eco systems in training and employing female youth(largely) to get employed in Apparel, Made-Ups and Home Furnishing sectors. The researches has done a study of Apparel training provided by one of the largest training partner in Odisha. It has tried to understand the training eco-system, facility available, experience of trainees and their journey from rural to urban location. It has also tried to capture some experience in terms training quality, employment opportunity and their social and economic changes.

Key terms : Skill, Sector Skill Council, Apparel, Made-Ups and Home Furnishing, NSDC

INTRODUCTION

Apparel, Made-Ups and Home Furnishing Sector Skill Council (AMH SSC) has been launched with a primary mandate of enhancing and to build a capacity in skill development. One of the salient features of the AMH SSC is designing of the training programmes, based on industry demands of different segments and to ensure that all successful trainees are certified through accredited assessment agency.

The AMH SSC was incorporated "To Develop a skills repository for the Apparel, Made-Ups and Home Furnishings value chain, To build an organization that can develop Standards, evaluation criterion and accreditation systems for providing multiple and varied technical skills in the textile sector including employ ability skills to both men and women, as well as challenged persons with regular and direct inputs from industry, Create opportunities for

"Training of Trainers "in both the content and pedagogy for imparting skill training for all workers engaged in the three chosen segments of the textile sector, Quality Assurance-Develop and promote a standardized, output oriented and quality assured affiliation and accreditation process and demonstrate sustainable business value through it, Focus on continuous improvisation of the training delivery value chain, i.e. training process, training content, trainers, curriculum design, industry endorsement for certification etc., Partner with training providers and guide them into becoming centre so excellence and innovation by utilizing the standardization in training, evaluation and certification developed by the SSC of the sector. Integration of Technology in Training, Development of a sector skill development plan and maintain skill inventory, Promotion of Resource Support Agency (academies of excellence), Establishment of a well-structured sector specific Labour Market Information System (LMIS) to assist planning and delivery of training."

India suffers from a large school dropout cases in women, particularly in rural India due to poverty, social stigma, inaccessibility to higher education, early marriage and engaging household work. This creates dependency of women in the society and leads to very poor quality of life. It has been experienced from ancient days that women get into some economic activity in design, fabric painting, stitching, making product from waste materials etc. and earn a little money to run the family. In order to provide employment opportunity, the organized skill training has immensely helped them to earn and lead a better livelihood. The skill training in Apparel, Made-Ups and Home Furnishings has given a wider prospect for job and self-employment.

LITERATURE REVIEW

The apparel manufacturer is responsible for all production activities, including the Cut, Make, and TrimCMT activities, as well as finishing. The firm must have upstream logistics capabilities, including trained manpower to run the production. This is a business model that focuses on adding design capabilities to the production of garments and precision manufacturing in volume production of same design. The industry is in need of skilled manpower to work in shifts and sometimes overtime in case of seasonal products. Most of the industry employs women worker that suits the nature of job. The Apparel industry suffers from high attrition due to migrated women workforce coming from rural area to work in apparel industry. But the industry absorbs large no. of women worker in turn empowering women of India.

Prasad and Purohit (2017), conducted a study on "Skill Development, Employability and Entrepreneurship through Make in India: A Study". The objectives of the study were to understand the success of Make in India movement on employability aspect through review of literature. The study is an exploratory research based on the secondary data and information collected from libraries, relevant books, journals, magazines, articles, media reports and Government portals of Make in India, Skill India, etc. The researcher adopted greater accuracy and in depth analysis of the research study based on available secondary data. The study gave an overall insights on status of skilling capability available and the skill gap and initiatives taken by Government of India to create an impact in producing skilled manpower and "make in India" project successful. The youth should be empowered with Technical and Vocational training along with Formal Education, to meet the Industrial manpower requirement. Despite various efforts and investments in shaping the skills of a huge labor force there are long way to go in achieving this mission and make it inclusive of our education systems. As a fast growing developing economy, apart from white and blue collar jobs, India also needs Grey collar- knowledge workers, with digitally aligned, innovation in solving social problems at the grass root level to support sectors like construction, agriculture and related trade. It is recommended to introduce vocational training as a part of School education. There is a great need for proper counselling to students at school level to decide their career based on academic standard and passion. Life skills training should be blended with technical skills to make youth more independent and accommodative to ever changing technology.

Ansari and Khan (2018), conducted a study on "Role of Education and Skill Development to Promote Employment in India". The objectives of the study were to analyse the status of current education with respect to skill development

and suggest based on the observations and analysis of the study. The study was based on secondary data collected from published reports, surveys, books, prominent sites, media reports etc. It is concluded that to sum up skill development for India is critical from both the socio-economic and demographic points of view. However, skill training is the important tool for reducing poverty, enhancing competitiveness and employability and to promote the self-entrepreneurship among youths. Now it is time to continuously examine the kind of skill training delivered and the need for changes/addition of new skill training in line with fast changing technology adoption in all sectors. To be more précised we need to move further into a knowledge-based economy, to promote industrial development and to achieve high economic growth, which requires huge investment in education and training for youth with a proper balance between them.

It is evident that there is lot efforts are being made at various level with focused attempt and support by Govt. of India to create employable women workforce to serve industry as well as to be self-employed irrespective of having or not the basic formal degree. Employment generation is the one issue other than that employability and productivity is another issue. Good news is that today, training in Apparel, Made-Ups and Home Furnishings has largely contributed in achieving "Make in India" mission too.

Research Gap

The skill training programme has a long term social benefits in creating employment through skill training. It is essential for all stake holders to have wider prospect of knowledge and feedback on the entire training activity;

- The quality of training programme
- Sustainability of this training in terms of pursuing same career
- Trainer's experience
- Employer views.

Research Objectives

Based on need and importance of skill training in our country the researcher tries to find insights that would help all stake holders to take appropriate action as deemed fit.

- Understand the logistics of Apparel skill training
- Highlight experience of women trainees faced during training and post job
- Make an impact assessment of the skill training in Apparel
- Suggest scope for improvement in training by training providers, funding agency and future participants

Research Design

The research is more qualitative and exploratory in nature. Researcher has administered a structured questionnaire to get specific data with reference to Research Objectives. The data received was compiled and presented in the form of graph/chart supported with data table.

RESEARCH METHODOLOGY

This research is explorative in nature. The researcher has studied the training Programmes and its impact on creating Employment and Self Employment of youths. The Study is in reference to Apparel skill training only. Research methodology is divided into five sections i.e. Section I contains Data Sources, Section II analysis of data collected from trainees.

Data Sources and Data Collection

The data required for the study was collected from primary sources on multistage random sampling method from trainees through a structured questionnaire and face to face interview. The secondary sources include journals, reports, websites and Government departments.

RESULT AND DISCUSSION

The analysis and interpretation of the various opinions given by the various respondents which were collected from the trainees are shown in the form of tables below.

Analysis and Interpretation

- The trainees were asked to respond on the reason for choosing Apparel training programme based on specific criteria.
- It was found that57% women join apparel training to get job. 23% of trainees are interested for self-employment, 9% for not havingopportunity to go for higher education.4% have an interest in apparel design and stitching and 7% due to their family pressure.
- A study was made to understand the mobilization process to identify and bring them to training organization. Each training organization follows different channel to create awareness about the training in rural area and get family support to leave them to join training and work in city.
- The study says 37% are influenced by their friends and equal % join out of their own interest. 12% get to know from media and 9% from local publicity. 5% join due to their family pressure to earn and support their family.
- The study was made know other opportunity for women, if they would have not joined apparel training programme.
- The study says, 32% of them would have done small traditional economic activity in producing and selling local products.34% of them would have joined higher studies and rest have no idea.
- The study was also made know trainees' experience in getting quality training which would make them for getting job or self-employed. The responses were taken regarding Over all Training quality, Training support,Training Design, Theoretical input, hands-on practice, classroom training, Training equipment/machine and Life skill training in the scale of Excellent, Good, Satisfactory and Poor. Almost 90% feedback was excellent and good. The trainees also appreciated the life skill training on digital technology, sanitization, etiquettes, working and living together, which was value added training for all skill trainees
- A study was made to understand the mindset of women on choosing and improving apparel training. 47% of trainees insisted on counseling their parents to allow them for this training, 28% for counselling to the candidates which indicates that the success of training lies on the attitude and motivation of parents as well as women candidate to leave their house and come to city for employment.
- A survey was made to find the aspiration of trainees post training. 72% of trainees are interested for job where as 28% want to go back to their native place and start tailoring shop and live with their family.

DISCUSSION AND CONCLUSION

The researcher found that Apparel training is one of the training opportunity for women to either go for job or to be self-employed. The training institute has given 100% placement opportunity for all women trainees after successful completion of 3 months training. The trainees are always asked to make uniform for their juniors at the end of training, which is pre-qualifying test for them to go for job in industry. The life skill training has largely helped them in understanding the industry environment of working and living together in working hostel. They are also made digitally savvy in operating smart phone to use apps for transferring money. They are trained on basic etiquettes, dressing sense, personal health care and safety.

It is evident that the Apparel, Made-Ups and Home Furnishings training has a greater impact in empowering women, be financially independent and for better livelihood. This is also supporting apparel industry in getting trained manpower. However challenges are in post married life in continuing job, which in turn creating high attrition in Apparel industry. The further research can be made to get the feedback from employer, parents of trainees and life after their marriage.

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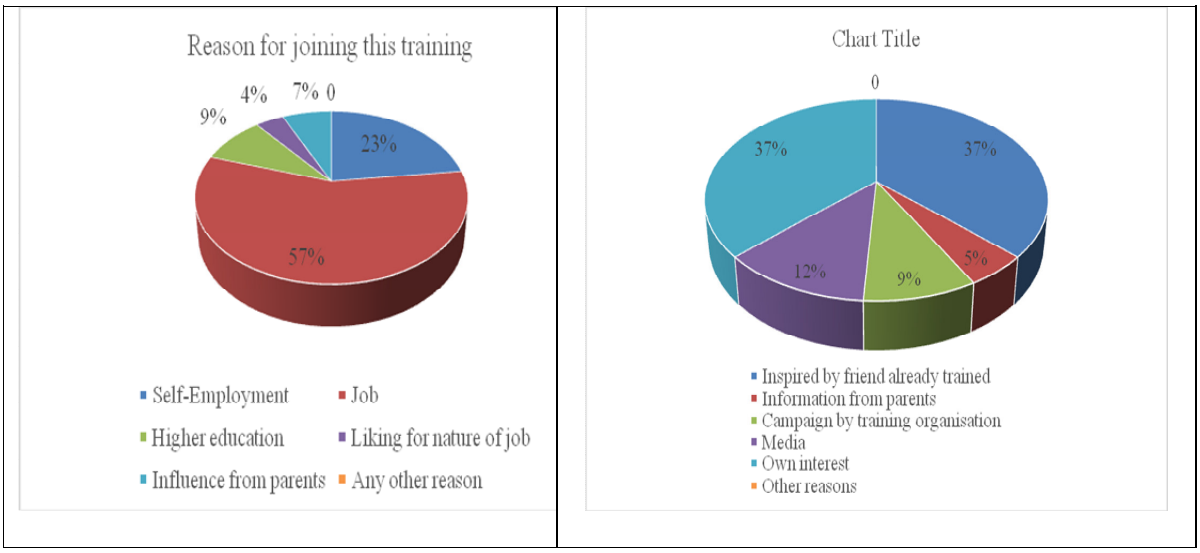


Chart Title
34%
32%
34%
0%
Create own small enterprise
Go for higher education
Daily labour work
No idea
Chart Title
70%
60%
50%
40%
30%
20%
10%
0%
Trainer support
Training design
Theoretical input
Practical input
Classroom facility
Training equipment
Life Skill Training
Overall Training quality
Excellent
Good
Satisfactory
Poor
Chart Title
50%
45%
40%
35%
30%
25%
20%
15%
10%
5%
0%
8%
0
8%
28%
47%
9%
Introducing new teaching pedagogy
Modifying training content
Improving infrastructure
Counselling youth to go for skill training
Counselling parents to allow their kids to go out of home
Creating awareness
Chart Title
0
0
28
72
Job
Self employment
Higher study
any other

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RESEARCH ARTICLE

Life Automobile Service; A Skill Training to Drive the Future of Youth

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ABSTRACT

The strong push for skill development in India has resulted in a fast-evolving landscape propelled by game changing reforms and policy measures under the banner of skill India. The report gives a brief outline of the history of skill development in India and highlights the main drivers for the big push towards skill development which are India's demographic dividend and the rapidly growth economy.India adds 12 million people to its workforce every year. By 2030, a third of words working age population is going to be from India. There are as many as 711 million people in India in the working age group of 15-59 years. With the majority requiring additional or new skills. India is a young and ambitious country with skills at the top of its agenda. The skill development policy also gives importance to promoting mobility of labour and encourages certifications and assessments that can ensure national and international recognition of acquired skills.Automobile Services training is an organised training that provides hands-on skill on service and maintenance of two wheelers. Traditionally youth are trained at automobile garage and gain competency by working for many years. It takes lot of time to acquire necessary skill to work on Automobile service centres or to start his own service centres. The researcher has a made study the responses toward the organised training and the quality of skilled manpower developed within a very short span of 3 months to 1year time.

Key terms :

INTRODUCTION

India is the youngest country among the world population. The major challenge today is to develop workforce with employable skills, through vocational education and also higher education to make India a developed economy. It is also essential to create employment opportunity for school dropout students, who couldn't have formal education and left with no choice than to be migrated unskilled labour.The country has 54% of the total population below 25 years of age and more over 62% of the population in the working age group (15-59 years), it strongly indicates that

India is one of the youngest country in world. By understanding global scenario, in coming 20 years, the current workforce in the technologically advanced world is projected to decline by 4%, but in case of India, it will increase by more than 32%. But the serious part is that as per the current statistics only 2% of the total workforce have accomplished skills development and vocational training in India. (www. pibphoto.nic.in). Considering globalization and rapid technological advancements, the skill development and skill capacity building is significant instrument to enhance the effectiveness and quality of skill force to optimize productivity and economic development.

Worldwide it has proved that the skill development is a vital driving force behind the economic stability and growth for the betterment of society of any country. Skill development is a very powerful instrument to empower individuals and improve their social recognition and dignity. This will lead to optimize economic improvements and creation of employment opportunities for aspiring Indian youth.The huge challenge is creating industry standards infrastructure and skilled trainers for skill training, with certain benchmark of quality. This is possible with Govt. policy, funding and support of industry to develop curriculum, provide internship and infrastructure in collaboration with training institutions.

REVIEW OF LITERATURE

Today Automotive Industry is known to be highly dynamic with continuous innovations, in design and development of auto components, changing the face of the industry. To cope up with such dynamic situation, skilling, re-skilling and up-skilling of the existing and future workforce is extremely important. The new jobs, however, are likely to move away from traditional manufacturing and instead be added in the areas of IoT, mechatronics, robotics, 3D printing, AI, machine and deep learning, analytics, virtual collaboration, automotive design, and computational thinking. The emerging and integration of the said technology, requires continuous reskilling of existing manpower working in service sectors and also creates avenues for new skilled manpower to serve the fast growing Automotive sector both in manufacturing and services.

It is evident that there are lot efforts are being made at various level with focused attempt and support by Govt. of India to create employable manpower to serve industry as well as to be self-employed. Employment generation is the one issue other than that employability and productivity is another issue. Currently about 26 million youth are getting into age group for employment every year with about 65% of them looking for jobs. Age and formal education degree is a constraint that affecting for skills development, because of social stigma. Good news is that today, there is no bar in gender for acquiring specific skill for their employment. To make "Make in India" project successful, youth of the nation should be empowered with formal education, technical and vocational training to meet the Industrial requirement as per global standards.

Research Gap

The skill training programme has a long term social benefits in creating employment through skill training. It is essential for all stake holders to have wider prospect of knowledge and feedback on the entire training activity;

- The quality of training programme and activity undertaken in supply chain; starting from mobilisation to post placement support
- The experience and Success story of trainees,
- Trainer's experience
- Employer views.

Research Objectives

Based on need and importance of skill training in our country the researcher tries to find insights that would help all stake holders to take appropriate action as deemed fit.

- To understand the supply chain of skill training services delivered by training organisation
- To highlight experience of trainees and their success story
- To make an impact assessment of the skill training in Retail and Hospitality
- To suggest scope for improvement in training by training providers, funding agency and future participants

Research Design

The convenience sampling method was used to collect primary data.

- Research Type –Descriptive type of Research
- Sample size – 60 respondents
- Trainees at GTET.
- Sampling Area – Bhubaneswar, Odisha

RESEARCH METHODOLOGY

This research is explorative in nature. The researcher has studied the training Programmes and its impact on creating Employment and Self Employment of youths. The Study is in reference to Retail and Hospitality skill training only. Research methodology is divided into five sections i.e. Section I contains Data Sources, Section II analysis of data collected from trainees.

Data Sources and Data Collection

The data required for the study was collected from primary sources on multistage random sampling method from trainees through a structured questionnaire and face to face interview. The secondary sources include books, journals, handbooks, newspapers, circulars, bulletins, working papers, reports, websites and Government departments.

RESULT AND DISCUSSION

The analysis and interpretation of the various opinions given by the various respondents which were collected from the trainees are shown in the form of tables below.

The trainees were asked to respond on the reason for choosing this training programme based on specific criteria. It was found that 73% students have joined this training to get job in an Automobile service sectors.

Motivation to join this Automobile training

68% of trainees had a self-motivation to join automobile service training and got enrolled to be trained and join this sector.

Quality of infrastructure and training support

More than 90% trainees appreciated the quality of training and rated in the scale of Excellent and Good, which a positive remark on training quality.

Quality of training and level of competency to get job

More than 85% trainees had viewed the training as a valuable input in building industry standard competency and will make them emp-loyable.

Feedback on improvement of skill training

The trainees emphasized on creating awareness about this training and counsel youth to get trained in new technology within a stipulated time and start earning.

SUMMARY AND CONCLUSIONS

The future of automotive industry is huge and volatile. The choice and need of customer is also increasing.The change in technologies, demands upgrading the skill of workforce and need specialist in the field of service. The focus has to be dual-mode training which includes the training and the practicing. The current study reveals that skill training in Automobile Services has been an attractive training model for the youth to get industry standard training in an organised set up. It also gives enough theoretical and practical insights on fault finding, assembling an engine and electrical fittings. The training creates wider opportunity to work in Automobile service centres as well as to start own service centre for any two-wheeler as the technology is almost same for all kind of two wheelers. Such training programme has a great demand in urban as well as rural sector, which protect migration of labour from village to city. Further it doesn't need any formal education to be trained and employed. Automobile training will continue to be one of the most preferred training programme for youth for passion and livelihood.

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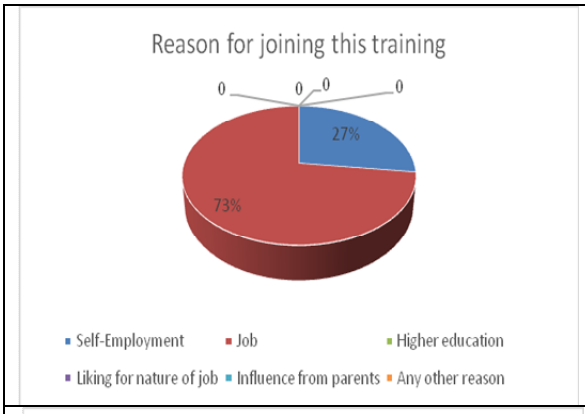
Reason for joining this training
0
0
0
0
27%
73%
Self-Employment
Job
Higher education
Liking for nature of job
Influence from parents
Any other reason

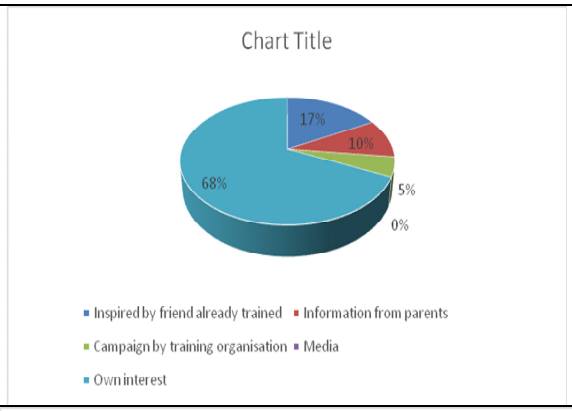
Chart Title
17%
10%
68%
5%
0%
Inspired by friend already trained
Information from parents
Campaign by training organisation
Media
Own interest

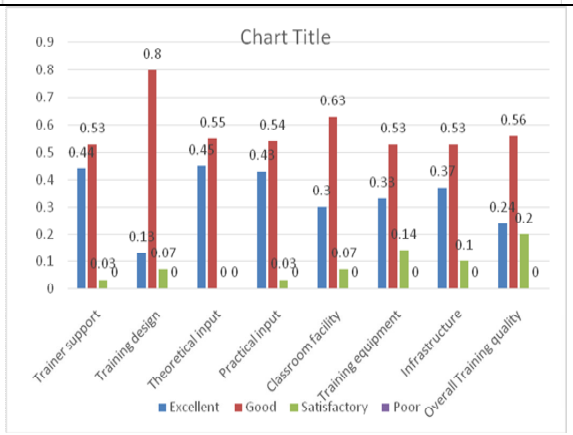
Chart Title
Trainer support
Training design
Theoretical input
Practical input
Classroom facility
Training equipment
Infrastructure
Overall Training quality
Excellent
Good
Satisfactory
Poor

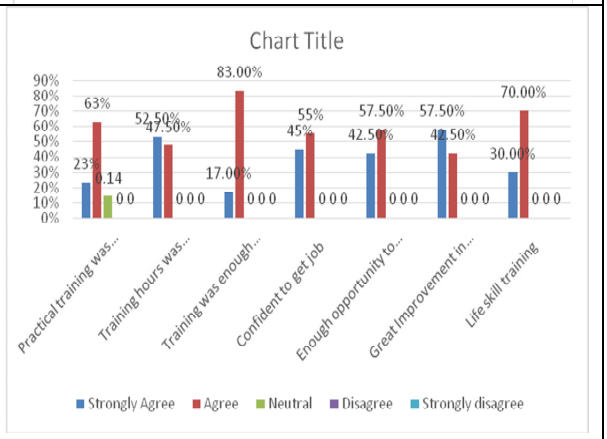
Chart Title
Practical training was...
Training hours was...
Training was enough...
Confident to get job
Enough opportunity to...
Great Improvement in...
Life skill training
Strongly Agree
Agree
Neutral
Disagree
Strongly disagree

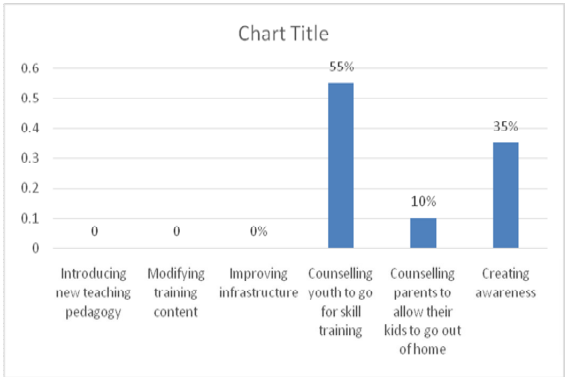
Chart Title
0
0
0%
55%
10%
35%
Introducing new teaching pedagogy
Modifying training content
Improving infrastructure
Counselling youth to go for skill training
Counselling parents to allow their kids to go out of home
Creating awareness

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RESEARCH ARTICLE

Change Detection Study Using Geospatial Technology and Remotely Sensed Data- A Case Study for Gajapati District

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ABSTRACT

Land use and land cover change were among the most substantial perceptible changes that are happening around us. Land use and land cover information in the form of maps and statistical data is very significant for spatial planning, land management and land utilization. With the changing times and growing demand on the availability of land use and land cover information, a standard classification system, precise description of land use and land cover and its categories, standardized data collection and mapping procedures across Indian region on different scales becomes relevant.Detection of digital change is the mechanism that helps to assess changes related to land use and land cover properties with respect to geo-referenced multi-temporal remote sensing data. It helps in recognizing changes that are uncharacterized by natural variability between two or more dates. An investigation was carried to define and measure the land use and land cover changes that have occurred in Odisha District Gajapati over the last 25 years using remote sensing and GIS technologies. Land is a natural resource of prime importance. A city not only increases by population but also by changes in the spatial dimensions. The development of rural areas has led to dramatic changes in land use and land cover. The importance of spatial data technology has been widely used in recent years, in particular the application of remotely sensed and geographic information systems (GIS).The present research explores land use and land cover in the district of Gajapati, Odisha using Landsat satellite images for the years 1991, 1995, 2000, 2005, 2010 and 2015. Supervised classification scheme is used to classify the different groups within the area of

study.The study showed that during the study period the built-up area in the district of Gajapati grew by more than fifty percentages on average. At the other hand, areas under forest, agricultural land, and open fields have decreased respectively by around thirty-eight and thirteen percentages.

Keywords: Land use/Land cover, spatial data, satellite, remote sensing, Image classification

INTRODUCTION

Land use defines the usage of land varying from area to area. In rural areas land use mostly includes forestry and farming [Annegarn H.J, Limpitlaw D, Kneen M.A][6]. In urban areas land use majors housing, commercials or industries. The type of physical and natural features present on the surface of the earth is known as land cover, e.g. Water body, forest, built-up area, etc. land use change, including land conversion from one type to another and landcover modification through landuse management, has greatly altered a large proportion of the earth's land surface to satisfy mankind's immediate demands for natural resources. Human population growth represents the primary driving force in land use change [M. K. Jat, P. K. Garg, and D. Khare][1]. Now a day's new technologies like satellite remote sensing and Geographical Information Systems (GIS) provides data to study and monitor the dynamics of natural resources for environmental management [Prafullaku.Panda and Tanuja G][2]. In the present study it has been mainly two types of data. These are topographic map and remote sensing data. Rural landuse land cover classification is still a challenge with medium or coarse spatial resolution remotely sensed data due to the large number of mixed pixels and spectral confusions among different land use landcover types [Latifovica R, FytasbK, ChencJ, ParaszczakJ][8]. Generally for rural areas, higher resolution images are more appropriate as the land cover structure is complex. Before the pre-processing and classification of satellite imagery began, an extensive field survey was performed throughout the study area using Global Positioning System(GPS) equipment[Sarma K., Kushwaha S.P.S][3]. This survey was performed in order to obtain accurate location point data for each land use and land cover class included in the classification scheme as well as for the creation of training sites [Chitade A.Z, Katyar S.K][4]. The satellite data was enhanced before classification using histogram equalization in ERDAS Imagine 9.2 to improve the image quality and to achieve better classification accuracy. In supervised classification, spectral signatures are developed from specified locations in the image. These specified locations are given the generic name "Training sites" and are defined by the user. Generally, a vector layer is digitized over the raster scene[Zubair, A.O][9]. The vector layer consists of various polygons overlaying different land use types. The training sites will help to develop spectral signatures for the outlined areas[Singh N.P, Mukherjee T.K and Shrivastava B.B.P][5]. Due to involvement of multiple data sets, we used latest technologies like remote sensing imagery, field survey, and existing study area conditions, here the study area is classified in to five categories, i.e. agriculture, built-up area, dense forest, barren land and water spread area. The study area covers 4325 sq. km and land use land cover changes were estimated from 1991 to 2015.

Detection of change is the process of identifying differences in the condition of an object or phenomenon by observing it at different times. Detection of Earth's surface features in a timely and reliable manner provides the basis for a deeper understanding of relationships and interactions between human and natural phenomena in order to better manage and exploit resources [Latifovica R, FytasbK, ChencJ, ParaszczakJ][7]. Due to a shift in land use patterns, however, land covers changes that affect biodiversity, water and other processes that combine to affect climate and biosphere. A detailed understanding of the impact of changes in land use/land cover pattern has become necessary for Gajapati district.This study was therefore undertaken to analyze the extent of human-induced landscape transformation in the affected areas of the district of Gajapatiby interpreting temporal remote sensing data using geographic information system (GIS) and cover types (dense forests, agricultural land, water bodies and barren land) to achieve the above objective.The rest of the paper is as follows: in Section 2, discussed briefly about the study area. In Section 3, have been describedthe materials and methodology. This is followed by resultand discussion in Section 4,accuracy assessment in section 5and conclusion of the paper appear inSection 6.

STUDY AREA

Gajapati district covers a total area of 4325 sq.km. The study area is located between 19°11'28.40"N and 84°11'8.56"E, (Fig-1). This is a district, the major part of which is hilly and with undulated topography. While the entire district has a population 5, 18, 448 the population density of the place is 116.66 persons per sq. km as per census 2001. The district has 10.19 percent population enumerated in areas classified as urban. Due to its agro-climatic conditions, Gajapati gains a large amount of its revenue through the agricultural sector. Also agro-processing and horticulture industries add to the economic wealth of this region.

MATERIALS AND METHODOLOGY

For this study, the orthorectified landsat satellite data was collected as per availability from United States Geological Survey website http://www.earthexplorer.usgs.gov. Satellite images used for this study were acquired from the sensors Landsat TM (Thematic Mapper), *ETM+ (Enhanced Thematic Mapper+)*on board Landsat 7. The study area falls under path row 140/47 of landsat. Details of satellite data used in the present study are provided in Table 1. Satellite images were processed using Erdas Imagine 9.2 software. Supervised classification method was used for mapping vegetation and land cover of the study area. This has been recognized as a most frequent method for remotely sensed data classification.In supervised classification method, the sample of known identify were used to classify pixel of unknown identify. Training sites in the images are generated to represent the typical spectral information of the land use and land cover classes (Forest, fellow land, built up area and water body)[Prafullaku.Panda and Tanuja G][2]. Training pixels are carefully chosen from the landsat images only after conforming their identify by comparing with toposheet, reference and local knowledge[Byeong-Hyeok Y, Kwang-Hoon C][10]. After the selection of training sites, the classification was run on the image using maximum likelihood classifier in ERDAS Imagine 9.2 software.
The brief methodology explained in the below flow chart (fig no-2.)

RESULT AND DISCUSSION

Two major steps include the land use and land cover (LULC) change detection method.

Independently classifying multi-data image and ii) Comparing individual LULC classes taking corresponding pixels in the multi date images.

Major changes were observed in the year 1991 the built up land covered 7.89 percent of the total area, this has increased to 10.8%, 14.44%, 18.7%, 20.68 %&21.8% in 1991-1995- 2000- 2005-2011-2015 respectively and the forest covered 48.72 percent in 1991 and decrease of 44.43%, 42.1%, 40.19%,38.32%&36.57% in 1991-1995- 2000- 2005-2011-2015 respectively and this change has caused the increase in water bodies from 3.34% to 3.32% due to water logging in the year of 1991 to 2000 and also decrease in trend 2005 to 2015. Agricultural land indicates in decreasing trend (25% to 18%) and barren land also varied in between 15% to 20% in the sub sequence years. It has been also observed that Mostly agricultural land converted in to settlement due to increase of population and urbanization.

LAND USE AND LAND COVER OF GAJAPATI DISTRICT

In 1991, forest constituted the largest category with spatial coverage of 48.72% of the total study area. Built up area with 7.89% and agricultural land and open fields, 25% of total area coverage. In the second time period, 1995 forest constituted the largest category with, 44.43% of the total study area. Agricultural land and open fields with 23.01% and settlement, barren land occupied second and third position respectively in terms of total area coverage. Figure-(3a-e) represent the changing pattern of land use and land cover of Gajapati district of study period. LULC of Gajapati district has undergone significant changes during the study period. Table 2: Percentage change in land use and land cover of Gajapati District.

Graphical representation of land use and land cover in GajapatiDistrict

The Graphical representation shows the land changes and its characteristics (Fig no5).Pie charts represents the changing pattern of land use and land cover of Gajapati District of study periodFig no 4 a to f. Land use land cover of Gajapati district has undergone significant changes during the study period. The changes in land use land cover over the past decade show an accelerated growth rate urban/builtup areas with increases of more than 15% in the year 1995 & 28% in 2015,representative of the population increases for this area. Agricultural areas and barren land have shown the greatest amount of decrease in this area, with dense forest decreasing by slightly more than 20%.

ACCURACY ASSESSMENT CLASSIFICATION

Accuracy assessment with the reference of the raw satellite images was carried out in this study. In the classification of maximum likelihood many pixels are often misclassified due to uneven data distribution [Prafullaku.Panda and Tanuja G][2]. Accuracy of classification should be done by ground truthing, or by physical appearance at the site of the study. But time is one of the big resistant in this situation, since you cannot calculate the past with the present.Therefore, acquiring better classification accuracy requires accuracy assessment of both infield and outfield. In this study outfield evaluation was carried out by random sampling of the reference image. To calculate the classification accuracy of each land cover image, the total process was taken by comparing the reference image with the classified image with some random point stratified random sampling.The rationale for using this sampling method is that each land cover class find equal probability of being observed 50 random points were used to assess the accuracy of each classified image. Some observations show the values of the '0' class, which are neglected. Data are summed up and qualified using the error matrix. Three different results of *accuracy-user accuracy, producer accuracy, total accuracy* was generated from the overall assessment which helps to understand the classification accuracy.The calculated assessment result of each classified satellite image from 1991 to 2015 shown in *Table-3*. Calculated total accuracy result for each satellite image (1991, 1995, 2000, 2011, 2005, 2015) given as 92.45%, 87.13%, 88.40%, 92.25%, 85.56%, 91.43%.

CONCLUSION

This paper focuses on improvements to the LU / LC in a rural area, using remote sensing data and GIS technology in Gajapati, India. The results clearly show that LU / LC changes during the period 1991 to 2015 were substantial. There is visible considerable expansion of built-up area. On the other hand, agricultural area is decreasing; water spread area, and forest areas. This study clearly shows the impact of population and their developmental activities on changes in LU / LC.This study proves how effective tool for urban planning and management is integration of GIS and remote sensing technologies. Quantifying LU / LC changes in the Gajapati region is very useful for environmental monitoring organisations, policy-makers and the public to better understand the local region.

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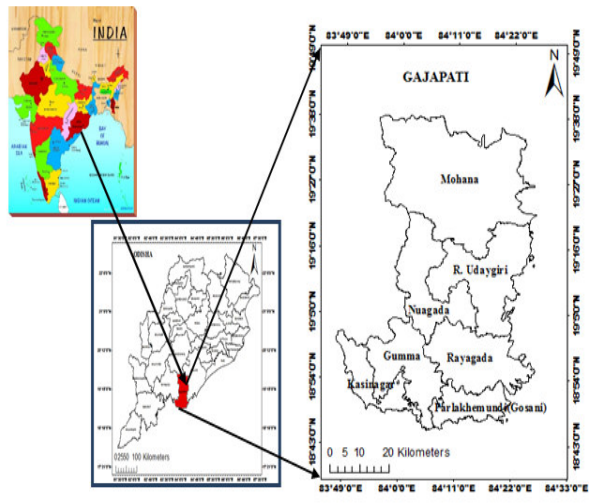

Fig. 1: Location map depicting the study area

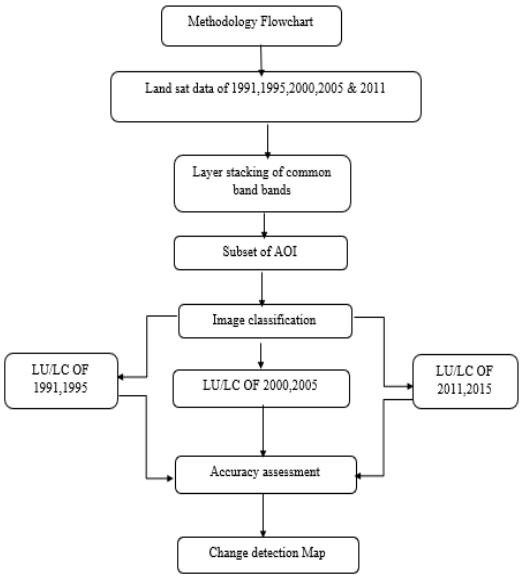

Fig-2 Methodology Flowchart

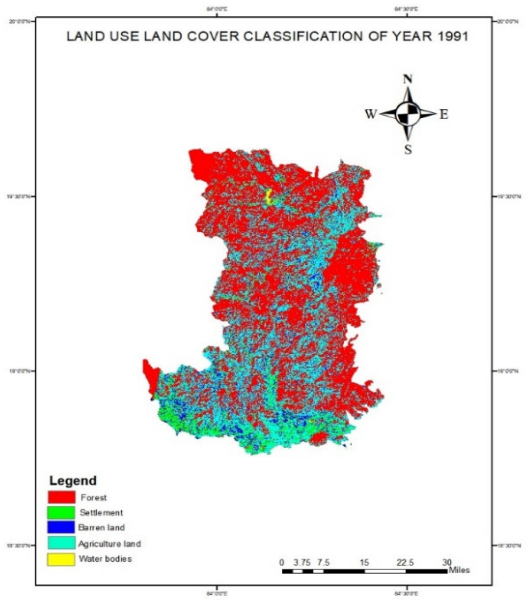

Fig 3a-LULC of Gajapati District of 1991

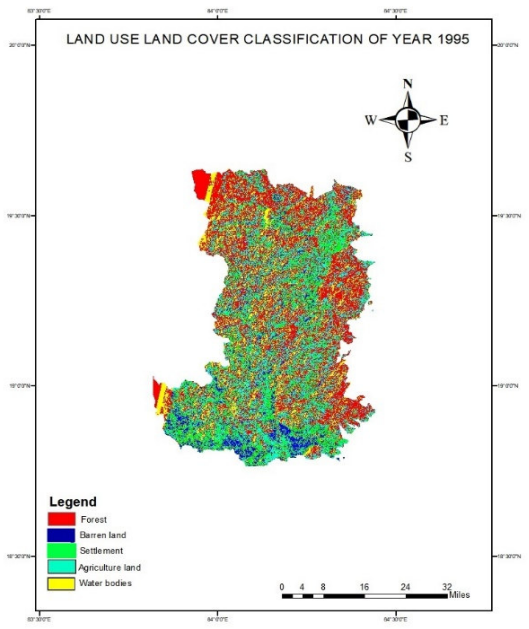

Fig 3b- LULC of Gajapati District of 1995

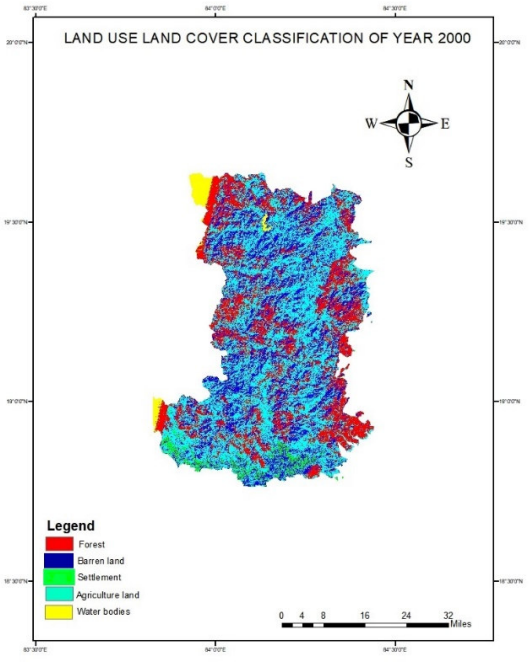

Fig 3c-LULC of GajapatiDistrict of 2000

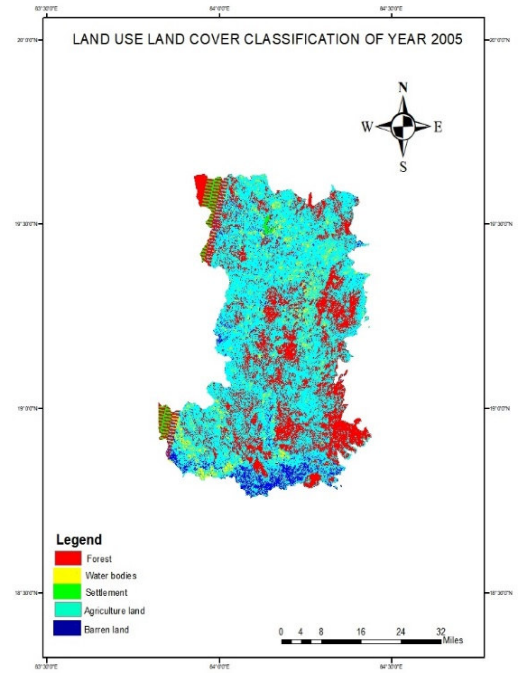

Fig 3d-LULC of Gajapati District of 2005

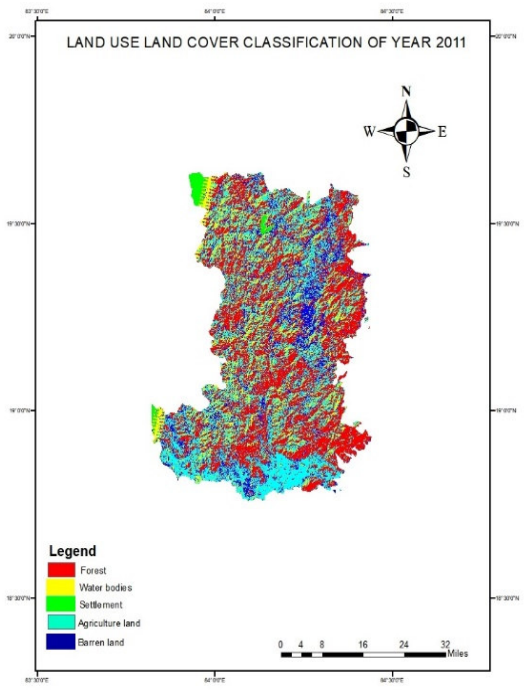

Fig 3e- Land use cover classification of 2011

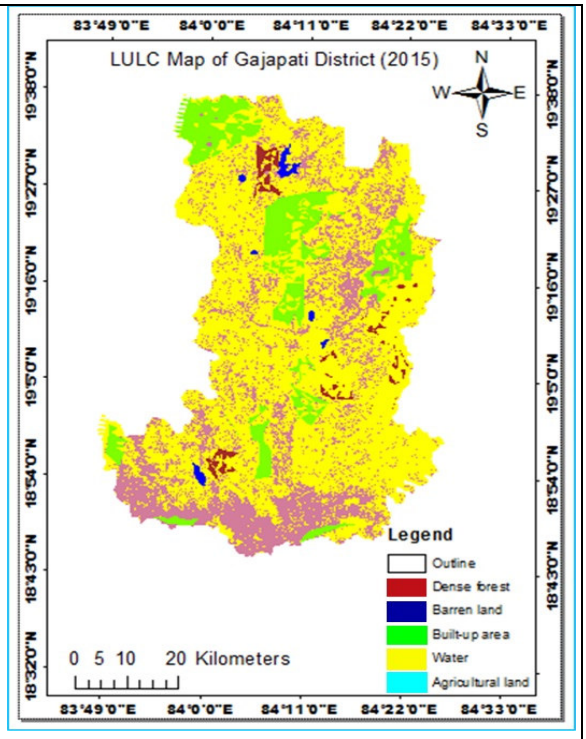

Fig 3f- Land use cover classification of 2015

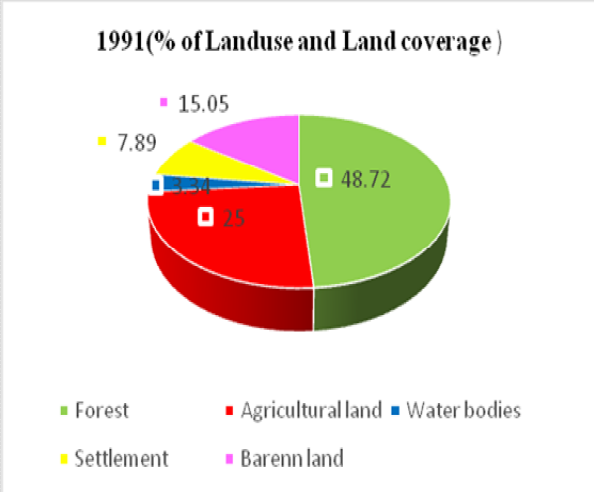

Figure 4a: LULC class percentages for 1991

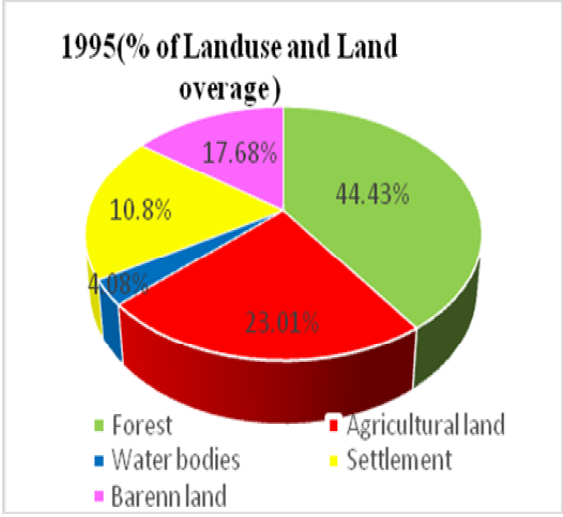

Figure 4b: LULC class percentages for 1995

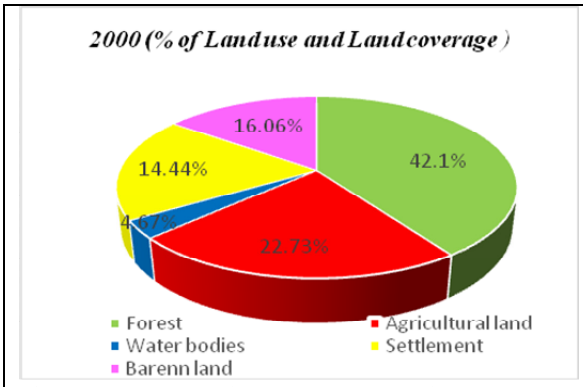

Figure 4c: LULC class percentages for 2000

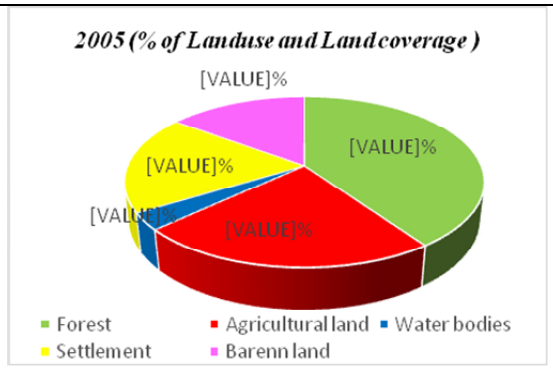

Figure 4d: LULC class percentages for 2005

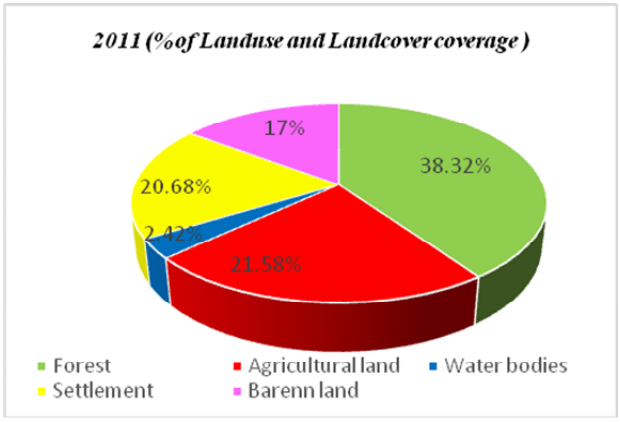

Figure 4e: LULC class percentages for 2011

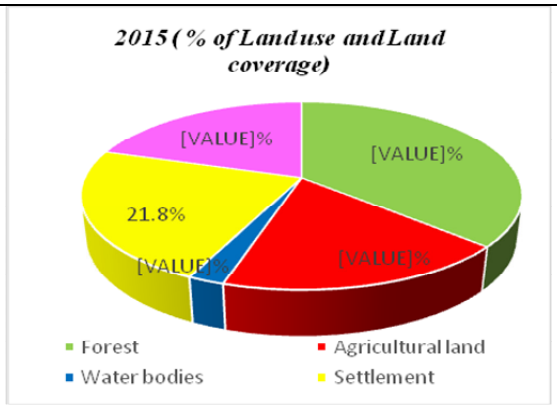

Figure 4f: LULC class percentages for 2015

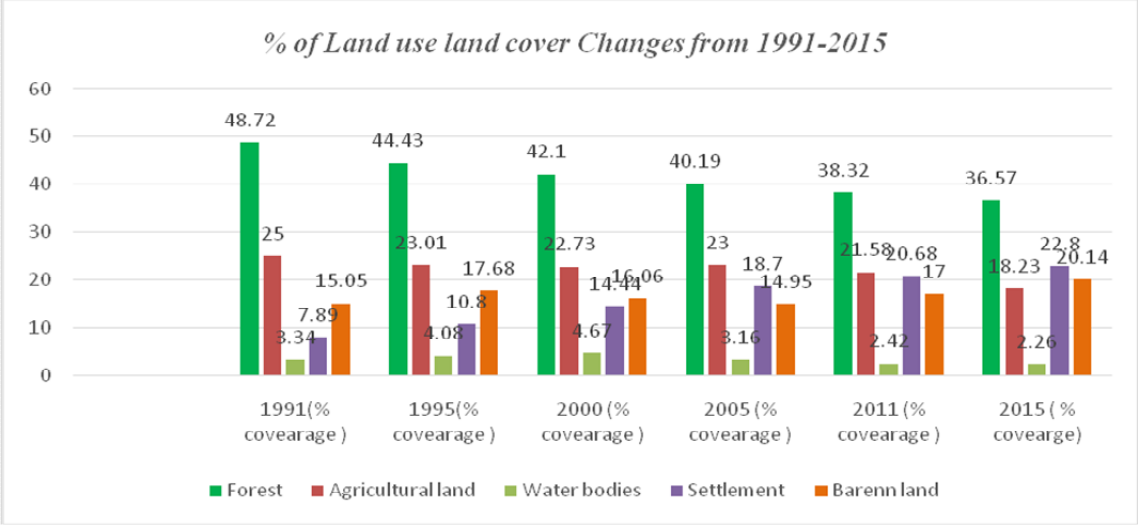

Fig no: 5 % of land use and cover changes during 1991 to 2005

Table-1:Satellite data used for the study

Used Data	Band	Date	Spatial Resolution
Landsat TM	7 Band	13-03-91	30m
Landsat TM	7 Band	11-02-1995	30m
Landsat ETM	7 Band	21-02-2000	30m
Landsat ETM+	7 Band+ Pan Band	13-05-2005	30m
Landsat ETM+	7 Band+ Pan Band	21-03-2011	30m
Landsat ETM+	7 Band+ Pan Band	16-05-2015	30m

Table 2: Percentage change in land use and land cover of Gajapati District

GajapatiDistrict land use land cover Change Detection Analysis							
Land use categories	**1991 % coverage**	**1995 % coverage**	**2000 % coverage**	**2005 % coverage**	**2011 % coverage**	**2015 % coverage**	**Remark**
Forest	48.72	44.43	42.1	40.19	38.32	36.57	During the study period all the categories showed both Positive and negative growth in area coverage, where the vegetation areas, agricultural land and open fields were converted into built up.
Agriculture land	25	23.01	22.73	23	21.58	18.23	
Water bodies	3.24	4.08	4.67	3.16	2.42	2.02	
Settlement	7.89	10.8	14.44	18.7	20.68	23.57	
Barren land	15.05	17.68	16.06	14.95	17	19.63	
Total	100	100	100	100	100	100	

Table 3: Accuracy assessment Table

	User accuracy					**Producer accuracy**						
Years	**Forest**	**Settlement**	**Barren land**	**Waterbodies**	**Agriculture land**	**Forest**	**Settlement**	**Barren land**	**Water bodies**	**Agricultural land**	**Overall accuracy**	**Overall kappa statistics**
1991	98.48	93.03	93.90	96.61	71.36	96.50	83.30	94.76	98.94	87.81	92.45 %	0.8872
1995	97.04	85.28	97.93	98.77	57.68	81.80	92.82	99.03	97.57	83.36	87.13 %	0.8184
2000	96.34	84.99	78.48	94.16	75.77	94.70	75.57	100	98.19	82.58	88.40 %	0.8363
2005	93.96	82.79	99.78	100	91.00	95.13	94.68	99.78	99.67	81.57	92.25 %	0.9004
2011	92.46	87.69	89.70	95.01	69.59	93.22	62.24	92.98	99.11	88.35	85.56 %	0.8185
2015	99.63	96.20	98.23	100	90.91	98.81	83.80	99.37	100	100	91.43	

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RESEARCH ARTICLE

Indigenous Traditional Knowledge (ITK) in Agriculture: Cases from Srikakulam District, Andhra Pradesh

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ABSTRACT

Across the nation, traditional knowledge system of agriculture varied from the society to society, which curved the history of food self- sufficiency. For centuries, farmers of the nation have stayed in the cave of deprivation, have maintained their distinctive culture of farming, have sustained on their traditional knowledge system. Historically speaking, almost all walks of life, tribal farmers stored their experiences. The experiences of farming stored since ten thousand years and most closely interacted with the socio-cultural lives of the farmers. Indigenous communities practicing farming are the conservator of traditional farm knowledge systems. The present study tried to explore a longitudinal data set on farm related Indigenous Technical Knowledge (ITK) system of the selected villages of Srikakulam, Andhra Pradesh. Multistage sampling has been adopted. The study draws attention on major factors of traditional knowledge systems. The study is based on Ex- post facto research design. The methods of data collection were quantitative and qualitative as well as participatory in nature and were aimed to seek answers to certain research questions. Participatory Rural Appraisal (PRA) and Observation are being the dominant methods. Keeping a foreside to the main objectives, the study emphasizes on understanding dialectics and dictum of ITKs in the context of family farming.

Keywords: Traditional Knowledge System, Indigenous Technical Knowledge (ITK), Family Farming

INTRODUCTION

The idea of farming appears to be ingrained in this earth since 10,000 years. Since inception, Indian agriculture is not merely an occupation, but it is the way of life which for centuries has been shaped outlook of life and livelihood of the nation. For a considerable period of time, farmers of the developing countries have remained in topographical variation, have kept up their particular culture of farming, have managed on family based farming, and attempted to defeat poor financial condition. Agriculture all through the world is up 'til now single most basic human activity. Despite each one of the advances of so called 'development', it is so far the primary source of sustenance and a basic origin of aspects and characteristic of society, whose produced substitutes are routinely not comparable to the normal components or all the more extravagant to make.

A few investigations by the farm dwellers, on experimentation premise have been occurring in the field of agriculture and associated fields for many years. They utilized accessible characteristic of Agricultural Experiences and contrived numerous advancements to expand the quality and amount of the yield of different endeavours, they had embraced. The information in this manner created throughout the years is dependable and has the property of ecologically friendly disposition. Such information is known as the 'Indigenous Technical Knowledge (ITK)'.Indigenous Traditional Knowledge (ITK) is a nearby information that is interesting to a given culture or society (Warren DM et.al 1989). The indigenous frameworks of yield creation developed over hundreds of years of social and organic advancement and speak to the gathered encounters of indigenous ranchers. The farm dwellers produce indigenous crops through information on ecological conditions and regular change without access to outer data sources, capital, and current scientific information (Maroyi, A. Improving et.al 2012).The commitments of indigenous and local information frameworks towards a superior comprehension of biodiversity and its sustainable use and the executives, has been recorded in the logical writing in numerous spaces: biodiversity conservation and wildlife management, customary marine resource management, rural development and agro forestry, traditional medicine and health, impact assessment; and natural disaster preparedness and response (IPBES et.al 2013). By and large, conventional knowledge has been orally passed for ages from individual to individual. A few types of traditional knowledge discover articulation in stories, legends, fables, customs, tunes, and laws (Kala, C.P. et.al 2012).

Objectives of the study

The study is the modest endeavour to highlight-

a) To identify the Indigenous Traditional Knowledge (ITK) in Srikakulam District of Andhra Pradesh
b) To trace out Social interaction pattern, ITK conservation and sustainability of family farms

METHODOLOGY

Research Design: The study was based mainly on Ex- post facto research design. The study was based mainly on Ex- post facto research design. Accordingly, after a thorough and meaningful formulation of the problems, specific objectives were decided. In the light of these objectives, an effort was made to make a thorough review of the relevant literature relating to the previous researches in this field.

The findings of this study have been discussed after analysis of the collected data through questionnaire and interview of the village dwellers on the subject and were subsequently summarized. The findings had been summarized after throwing light on all the major aspects of the study. The conclusion and the suggestions were made to make the agricultural development possible through judicial utilization of ITK.

Locale of the study area: The study was conducted in the selected areas of Seethampeta, L.N.Peta, and Polaki blocks of Srikakulam district, Andhra Pradesh.

Sampling procedure: Purposive- Snow ball sampling method was adopted.

RESULTS AND DISCUSSION

Documentation of the Indigenous Traditional Knowledge (ITK) in Srikakulam District of Andhra Pradesh

The inception of indigenous information can be followed back to the antiquated period. Individuals utilized such information from age to age for their work in an unaccounted way. There is no composed archive for recording and storing of such information. It is found that such information/ knowledge framework is fundamental for agricultural development. It must be accumulated and reported through a specific network.

Here is the list of ITKs, collected during field study

1. Farmers use Mahua (*Madhuca indica*), Mustard and Neem Cakes to maintain the soil fertility and moreover to protect crop from soil born insects and diseases.
2. Decomposed leaves, crop residues and forest waste materials are mixed in the field followed by harrowing by bullock drawn blade harrow.
3. Forest residue and soils broadcasted over the field and deposit during rainy season to increase the soil fertility.
4. Dhenkur system for irrigation: This is a traditional method of irrigation in which farmers irrigate field with the help of bucket attached to wooden handle. It requires continued/ permanent manpower (labour) to operate irrigation.
5. Farmers walk around the field and press the soil by foot to ensure the ploughing condition.
6. Hal: Deshi wooden plough used for ploughing or cultivation.
7. Hundi and Tokani: Broadcasting method of sowing of seeds is most popular among the tribes. During broadcasting the seeds are kept in Hundi (soil made pot) and Tokani (bamboo made pot).
8. Jarkati: Used for harvesting purpose.
9. Dusting ash to control aphids
10. Beating drum in standing crop to scare birds
11. Ants running from down to up with their eggs indicates heavy rain.
12. If rainbow appears in the east in the evening or west in the morning, it will rain.
13. Clouds of dark brown colour cause heavy rains for a fortnight.
14. Dragonfly flying near the ground is an indication of rain.
15. In storage structure some rural folk have “Dhusi” made of paddy straw, which is a low cost device and help in storage of grains/seeds for longer duration.
16. To prevent termite problem, mucidi leaves (*Strychnosnux-vomica*) are applied as green manure in direct sown paddy.
17. Onion, neem leaves, common salt and turmeric slices ensure the safely storage of grains.
18. Tentemu leaf (*Cassia tora*) and jeelugu (Caryotaurens) twigs are incorporated during second ploughing for better decomposition and utilization to improve soil fertility.
19. Tribal farmers apply 50 kg of neem cake in paddy field during puddling to control insect pests and improve soil fertility.
20. Laying of stone bunds around the fields across the slope for preventing soil erosion and for conserving moisture is practiced.
21. Spray of Neem extract solution to control leaf minor insects.
22. Tribal farmers dust the mixture of kitchen ash and turmeric powder on vegetables to prevent the aphid attack.
23. A man like effigy made up rice straw wearing a dress and head is covered with an earthen wear made like a human head is used to keep in the centre of the field. The birds fly away because of human appearance in the field.

24. A man made structure known as "Kakbhagoda" is used for protection from birds.
25. A man made structure known as "Mairamadicha" is used for supervision of crops as well as protection from animals.
26. By use of bamboo stick for threshing.
27. By moving bullocks on the circle over the crop, spread in the threshing floor.
28. Uprooting by hand for weeding.

Along with these, some more ITKs were identified through FGD. Here lies the detailed transcription.

Social interaction pattern, ITK conservation and sustainability of family farms

Thus of a complete investigation of different government and non-government institutions connected with the advancement of agricultural improvement it was recognized that there were essentially five classes of institutional systems that could have a beneficial outcome in the same. The parts of the current institutional system are as per the following-

- Government Institution and professionals (92= KVK, 97= BTM, 100, 101= Block level organization)
- NGOs (93= Society for Participatory Action and Reflection , 94= TSCSR, 95= Tagore Society, 96= Jan ChetnaManch)
- Input dealers (91, 98,99)

Blue circles were depicting the institutions. Red circles were the respondents. Green arrows were depicting reciprocal relationship among the respondents. Evaluating the sociogram depicted here, it was found that 94, 95, 96, 92 were the most frequently chosen institution. Out of these, 94 and 95 had highest impact in community. The size of the blue boxes is directly proportional to the impact of the institutions.

The initial phase in building limit with regards to systems administration in rustic groups will begin from helping the provincial individuals to comprehend their administration comprehend and envision their current systems (Douthwaite et al., 2006). Here it is clear from the Figure 4.2.4 that farm related information is mostly spread by NGOs, KVK (KrishiVigyan Kendra)s, BTM (Block Technology Manager)s and agricultural input dealers.

Here, NGOs and agricultural input dealers are playing most vital roles. It is because of their ability to penetrate in grassroots level. The data, obtained from sociometry, has been quantified and analysed through UC NET.

NGO's sort out preparing programs for the wage creating exercises (IGA). A portion of the NGOs' capacities and points of interest, as indicated by Streeten (1997) are:

- They are great at coming to and assembling poor people and remote groups;
- They cause enable needy individuals to pick up control of their lives, and they work with and Fortify nearby establishments;
- They do ventures at lower expenses and more effectively than the administration organizations and (4) they advance supportable improvement.

From sociograms, obviously a large portion of the expertise advancement programmes for farmers were conceived by the nearby NGOs of the review range. KVKs (Govt. Establishment) had less effect than the NGOs. Different establishments like Bank and Input Dealers have no effect on aptitude advancement preparing.

CONCLUSION

It may be finished up by saying that in one hand Traditional farming is exceptionally powerful instrument for improving the financial situation of farm dwellers regardless of their types (marginal, small and for banishing joblessness and underemployment) by judicial utilization of the resources. During this study, 28 ITKs were

identified. From Sociograms, obviously a large portion of the expertise advancement programmes for farmers were conceived by the nearby NGOs of the review range. KVKs (Govt. Establishment) had less effect than the NGOs. Different establishments like Bank and Input Dealers have no effect on aptitude advancement preparing.Effect of common society and Government Organizations are continuously recognized as authority by exchange of innovation. The foundations are considered as the administrators of spreading new advances. Hence, traditional knowledge system should be blended with mainstream agriculture.

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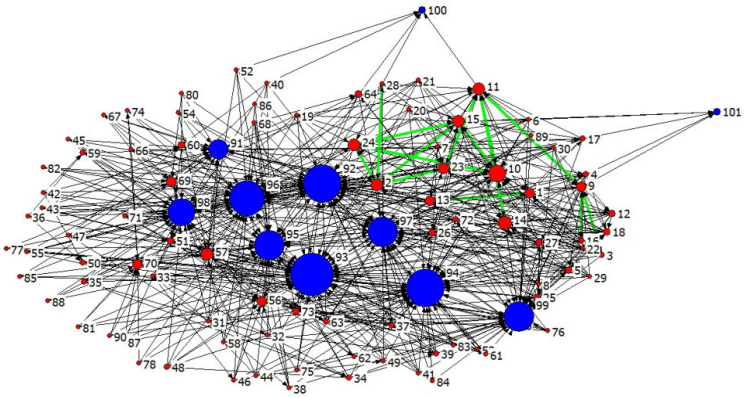

Fig 1 Social interaction

Table 1 District wise distribution of the respondents

Distrct	Block	Village	Respondents
Srikakulam	Seethampeta	Gajili, Kadagandi, Kusimi	90
Srikakulam	L.N.Peta	Chorlangi, Karakavalasa, Pusam	90
Srikakulam	Polaki	Ampalam, Koduru, Rajapuram,	90
Total Respondents			**270**

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RESEARCH ARTICLE

Ethnographic Analysis of Family Farms: A Case of East Singhbhum, Jharkhand

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ABSTRACT

Since time immemorial, Indian Agriculture has paved the path of culture. The idea of farming appears to be ingrained in this earth since 10,000 years. Since inception, Indian agriculture is not merely an occupation, but it is the way of life which for centuries has been shaped outlook of life and livelihood of the nation. For a considerable period of time, farmers of the developing countries have remained in topographical variation, have kept up their particular culture of farming, have managed on family based farming, and attempted to defeat poor financial condition. The present study tried to explore a longitudinal data set on farm related Indigenous Technical Knowledge (ITK) system of the selected villages of Srikakulam, Andhra Pradesh. Multistage sampling has been adopted. The study draws attention on major factors of traditional knowledge systems.Agriculture all through the world is up 'til now single most basic human activity. Present study is intending to ventilate the ethno-culture of family based farms. The study was set in the background of Chotanagpur plateau of Jharkhand. It considers tribal farms as the unit of ethno-centric agricultural system.

Keywords: Family Farming, Ethnographic Analysis, ITK, Jharkhand

INTRODUCTION

Mazyer and Roudart (2012) explained the history: if humankind somehow managed to permit each developed biological system of the planet to lie neglected, each would rapidly come back to a condition of nature near that in

which it existed 10,000 years ago. Wild vegetation far more grounded than those current today would overpower developed plants and tamed creatures. A predictable reaction of farming extension and strengthening has been the fracture and disconnection of normal natural surroundings inside an inexorably inadmissible lattice for some species (Donald et al., 2001). Natural surroundings discontinuity and its belongings prompt a scope of environmental and biological system changes. Among these, biodiversity characteristics, for example, species arrangement, group structure, populace elements, conduct, reproducing achievement, and individual wellness are adversely influenced (Silva and Pontes, 2008). A few investigations by the farm dwellers, on experimentation premise have been occurring in the field of agriculture and associated fields for many years. They utilized accessible characteristic of Agricultural Experiences and contrived numerous advancements to expand the quality and amount of the yield of different endeavours, they had embraced. The information in this manner created throughout the years is dependable and has the property of ecologically friendly disposition. Such information is known as the 'Indigenous Technical Knowledge (ITK)'. Indigenous Traditional Knowledge (ITK) is a nearby information that is interesting to a given culture or society (Warren DM et.al 1989). Spradley (1973) defined the methodology of 'Ethnographic' Analysis. It was used by the anthropologists. According to him, it is the work which describes the culture. Again he added that the goal of ethnographic analysis was to synthesize parallel way of life from the native point of view. In this sense, 'Ethnographic analysis of Family Farms' anticipates to express the culture of farm and farming.

METHODOLOGY

Sample size: 270 samples were drawn by using Multistage Purposive Sampling.

Sampling Design: From the district, 3 blocks having >60% tribal population had been selected. Thereafter, 3 villages were selected from each block. After that, 30 farmers were selected from each village.

SELECTION OF THE STUDY AREA

1. **Selection of the district:** Jharkhand is comprised of 27 districts. Out of this one district namely East Singhbhum was conveniently selected for the present study.
2. **Selection of the block:** There are 11 blocks in Deoghar district. Out of these 11 blocks, three blocks namely Ghatshila, Patamda and Baharagora block were purposively selected for the study.
3. **Selection of village:** Darisai, Bodhpur and Bhamradih villages of Ghatshila block, Dongagarh, Dhatkidih and Loraidoongri villages of Patamda block, Jarabani, Pochakhuli and Satpati villages of Bharagora block were selected. Figure 1 describes the framework of the Ethnographic Analysis of the Family Farms.

The steps in 'Ethnographic Analysis of Family Farms' using the observation, discussion as adapted are-

- Personal Interview of the sample farmers. Visit the farms with them.
- Discussion with the farmers.
- Topic of discussion- Land classification, Land Management, Cropping Pattern/ System, Farm Management, Agricultural operations etc
- Verification of information.
- Sketching and documentation of important operation and facts.

RESULTS

Outcome of the investigation

Traditional land Classification: In accordance with the description of space utilization pattern of the farms, land classification is one of the most important concerns. In keeping with the specific characteristics of the land, it is classified into two major segments- Upland (Local name- Tanr) and Low land (Local name- Doin/ Don). Based on

some essential characteristics, Tanr is again divided into three parts- Tanr I, Tanr II and Tanr III. Doin/ Don have three more divisions- Don I, Don-II and Don III. Detailed description of 'traditional land classification' is presented through table 1.

Identified indigenous farm practices

Table 2 depicts various identified indigenous farming practices under each family farm.

DISCUSSION

Indigenous soil management practices: Conventional farming is frequently viewed as a stage between the neighbourhood chase and-assemble rehearse, which furnishes groups with subsistence levels of nourishment, and the acts of present day agribusiness, utilized for large scale manufacturing of sustenance for worldwide dispersion. Customary rural methodologies are not down to earth for mass sustenance generation, but rather represent a considerable measure of neighbourhood nourishment creation in the creating scene (Jeeva, Laloo and Mishra, 2005).

Preparation of land: Preparation of land is critical to guarantee that the rice field is prepared for planting. Generally 4-5 ploughings are used for tillage operation. A well prepared land controls weeds, reuses nutrients, and gives a friable soil mass for transplanting and an appropriate soil surface for direct seeding.

Furrow opening: This type of operations were done to prevent water loss and to store the rain water. The locale of East Singhbhum comes in the discrete precipitation range and in the absence of legitimate administration framework the greater part of the water goes squander as spill over. Figure 4.1.2.17 depicts furrow opening structure for water conservation

Summer ploughing: It is mostly done in low lands (*Don*). It raises the water holding capacity of the soil and reduces water runoff. It also helps to control insect-pest infestation in field. Singh and Sureja (2006) opined that it exposes egg end spores of insects to hot sun light. As a matter of fact, incidents of pest infestation were reduced by this cultural method. They also told that it was one of the most popular ploughing methods.

FYM based manuring: The farmers of the study area used to store cow dungs in handmade basket or in the corner of field (Heap method). Well decomposed cow dung is good for soil health. In study area, peoples were using FYM since 50-60 years.

Small water holding structures: The study canvassed the findings on traditional water management structures of the study area. In this portion, it was documented how the farm dwellers used to manage the indigenous water holding structures. From the study, it was revealed that they had micro water holding structures like- Doba/ Pukra, Happa.

Doba is a micro water holding structure which occupies 1-2 ha land. Onset of monsoon, it conserves 4-6 m^3 water. Dey and Sarkar (2011) also found 'Doba' as a part of traditional water harvesting structure. They explained that In spite of the fact that on a normal 140 cm precipitation is gotten in Chotanagpur level, water is the absolute most essential limitation in foundation of agro-ranger service. Simultaneously, each Doba structure with 4.5 m3 limit (3.0 m length, 1.5 m broadness and 1.0 m profundity) has been developed for gathering of water before the onset of rainfall. They also opined that the drainage water from the fields which streams in little rivulets is gathered by developing a bund in the lower spans of the rivulets and where water can be put away. Contingent on the accessibility of seepage water, comparative bunds might be built at many focuses along the length of the rivulets.

Happa, a water holding structure, was made through excavating the field. Jana (2011) opined that the sides of a Happa were ventured with slant of 1:1 to such an extent that both animals and human can get to the water of Happa effectively. A Happa was developed by the side of rural field of a rancher with normal length of 45 ft, broadness of 50 ft and profundity of 12 ft.

Along with *Happa*, roof water harvesting was also done by the farm dwellers. By using 'Dugout' structure, some farmers were harvesting rain water. Some NGOs and GOs were promoting the structure in the study area. Water harvesting was also done by field bunding and terracing.

Threshing and Winnowing: Winnowing is an indigenous method to segregate rice grains from chaff. Chaff is the scaly cover of paddy grain. With the help of '*Kulha*' winnowing is done by blowing off the chaff. Threshing helps to remove grains from straws. Winnowing also helps to wipe out stored grain pests like- weevils.

Plot levelling by indigenous wooden leveller: For levelling the plot traditional leveller ('Soohaga') were used. It is a bamboo made instrument, having wooden plank.

Crop residue mulching: Crop residues are the by-products of the crops. In the study area, crop residues were used for mulching. They were practicing this type of mulching since 15-20 years. Mostly paddy residues, straw, tree leaves were used for mulching.

Stone weir/ bunding: Stone bunding is a traditional method of soil and water conservation. These bunds are made with locally available stones across the slope. During high rainfall, it helps to store water and to stop soil erosion. To stabilize their bunding people use to plant some bushes and plants there. **Stone cum vegetative**bunding was also popular in the study area. **Stone cum earthen bunding** includes building stone bunding at the construct took after by earthen bunding with respect to the top. In some cases, in stone bunding, soil is filled into work as an establishing operator.

Pest and disease management: Other than hand weeding to control weeds, some farmers often used kerosene and neem oil to control the weeds. Kerosene was also used to prevent pest infestation. Cultural methods like- water logging, trap cropping were used to control termites and other crops.

Indigenous instruments for fishing: There were several traditional fishing instruments; out of which two were documented.

Taap/ Machchibaksha: It is made of bamboo sticks. Conical shaped baskets are prepared by the local fishermen. At the top of the basket, one ring is attached. Height of the instrument is 80-90 cm. At the end/bottom of the basket, there is another ring which is bigger in size. These types of fishing instruments are generally used in shallow depth water bodies.

Major benefits of these kinds of conical baskets are- 1) Cost of production is low (Rs. 90-150/-), 2) User friendly and 3) Easy to carry.

Ghanj: This is a traditional fishing trap which is prepared from bamboo sticks. It is tied with nylon threads and looks like 'V' shaped folded mat. It is mostly used in the weed infested ponds where net is not useful.

CONCLUSION

Everybody now consents to the way that expanding populace and land discontinuity will influence human oversaw frameworks also. Cultivating frameworks, specifically, is helpless against such changes. Since living has turned out to be more mind boggling than some time recently, human need, particularly nourishment propensities, has likewise been moving quickly and among the general population agreement is progressing that by itself cultivating can't meet these developing requests of the general population by harvest development as it were. It needs enhancement with different endeavors in the cultivating frameworks to adapt up to this change.

Family farms allude to the homestead where in at least two differing financial endeavors are coordinated with ranch assets for accomplishing their more full use, acknowledge most extreme benefit and guarantee returns. Along these lines, the essential goal of the Farming System is to enhance quickly the financial states of individual homestead families by expanding change, heightening and expansion of various undertakings and generation methods keeping

in view the most recent advancements, requirements forced by assets, social taboos and the earth. Keeping this in view, the present review was embraced with the accompanying destinations.

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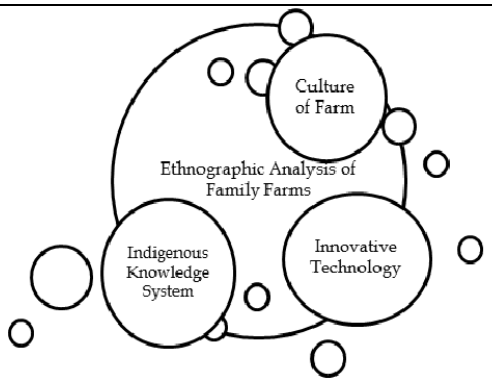

Figure 1 Ethnographic analysis of Family Farms: Framework

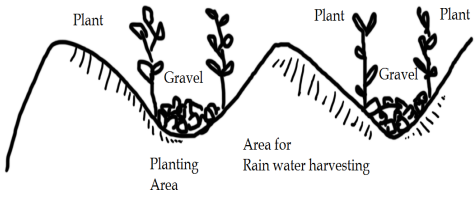

Figure 2: furrow opening structure for water conservation (SketchSource- Researcher's field note book)

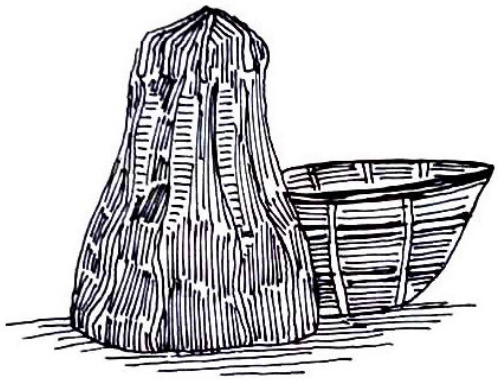

Figure 3: Traditional handmade basket- *'Tokri'* (SketchSource- Researcher's field note book)

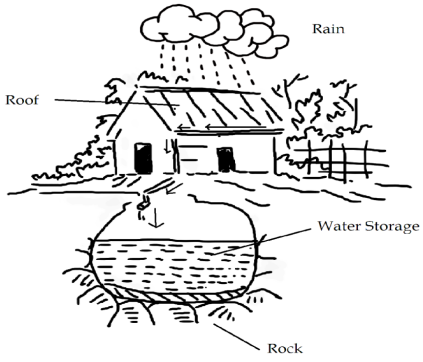

Figure 4: 'Dugout' structure for water harvesting (SketchSource- Researcher's field note book)

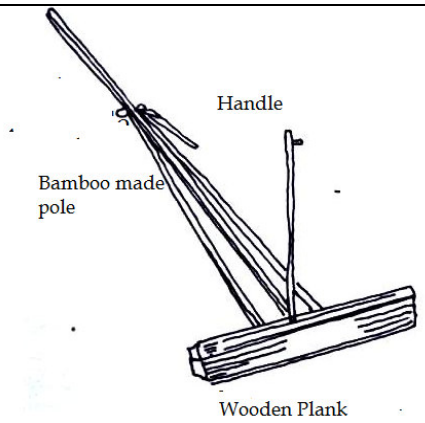

Figure 5: 'Soohaga' – indigenous leveller (SketchSource- Researcher's field note book)

Figure 6: 'Taap' – indigenous fishing instrument (SketchSource- Researcher's field note book)

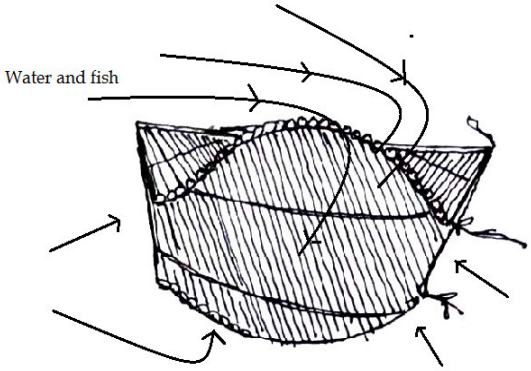

Figure 7: 'Ghanj' – indigenous fishing trap (SketchSource- Researcher's field note book)

Table1: Traditional land classification

Revenue Classification	Sub-Category	Character	Indigenous Name	Major Crops
Tanr (Upland)	Tanr III	Highest strip of upland, Worst soil fertility, Sloppy, Lumpy texture	*Tanr*	Not suitable for cultivation, Mostly human habitation
	Tanr II	Next strip of Tanr I, Erosion prone, poor soil fertility, coarse texture	*Gora Jameen*	Some vegetables (rare)
	Tanr I	Just above the Don III, Soil fertility better, water holding capacity is better than Tanr I and II	*Bari Jameen/ Bhumi*	Mostly used for vegetable cultivation, Rice (broadcasting)
Doin/ Don (Low Land)	Doin/ Don III	Superficial low land, Extension of Tanr I	*Charura Bari*	Rice
	Doin/ Don II	Fertile low land	*Tarkha Bari*	Rice (suitable)
	Doin/ Don I	Lowest strip, Most fertile land	*Ghogra*	Rice (suitable)

Table 2: Indigenous farming practices in Family Farms

Sl. No.	Indigenous farming practices
1	4-5 times ploughing before sowing/ planting (Paddy)
2	Furrow opening for rain water harvesting
3	Summer ploughing
4	FYM based manuring
5	Small water holding structures- *Pukra/ Doba, Happa*
6	Thrashing and Winnowing
7	Plot levelling by indigenous wooden leveller
8	Crop residue mulching
9	Stone weir/ bunding (to stop soil erosion)
10	Paddy threshing by bullock
11	Live bunding by cactus
12	Sun drying before storage of paddy
13	Repeated monsoon ploughing
14	Stone-cum- vegetative bunding
15	Use of Kerosene to prevent weed infestation
16	Gravel and sand mulching
17	Clod braking by indigenous wooden instrument
18	Field bund
19	*Ghanj*, *Taapi*(Bamboo made busket)
20	Rainfall/ weather related knowledge

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RESEARCH ARTICLE

Role of Extension Workers and Institutions in 'Agricultural Technology Transfer'

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ABSTRACT

Man/Woman, by virtue, is a social animal. People are interdependent in a society. Various factors and web of several relationships created a symbiotic relationship among the dwellers of a society. This relationship, then, depends on the fecund recital of the interaction pattern. Extension Workers ensure the arrangement of transferring new agricultural technology and thought to the farming community for sensitizing them. The specialists, hence, not just advises farmers to enhance their production and set up an orientation, additionally inspire them to use new farming technologies according to their conveniences.Extension worker has a critical connection between research associations and farmers. In a settled farming system, small farmers are made fit for utilizing new innovation and extension workers are relied upon to disclose to the farmers the mechanical focuses required in the utilization of new agrarian advancements.This paper has campaigned the analysis and discussion of role perception and role consensus of extension workers. It has an impact on overall role performance of the extension workers.

Keywords: Extension agents, Family Farming, Sustainable Livelihood, Network Analysis.

INTRODUCTION

The poor village dwellers are capacitated because of different reasons, for example, the greater part of them are socially in reverse, ignorant, low inspiration and poor monetary base. Separately a poor is poor in financial condition as well as need access to the learning and data, which have turned out to be most imperative parts of today's advancement procedure. Be that as it may, in a gathering the poor can defeat a hefty portion of these shortcomings (Talukdar and Dutta, 2009). Institutions and NGOs frequently assume a crucial part in the mass preparation, and usage of FS Models. They have powerful grass root level infiltration. To execute inventive Agricultural Technologies, NGOs have basic part of making mass refinement. Bose et al. (2003) opined that they would work with government, state, and nearby pioneers to propel the objectives… . NGOs likewise have specialized and human asset ability, which they can use to help decipher very mind boggling logical ideas which controllers, lawmakers, and individuals from people in general can promptly get it.

Organizations are sharpening essential partners (women and men farmers) and they could assume a huge part in starting a SHG and furthermore masterminding specialized ability improvement programs for the SHG individuals. Women/Farmers are regularly ready to grant specialized information and expertise. A few NGOs are likewise attempting to create promoting chains during the time spent building up on a venture by them for greater manageability.

Networking and livelihood framework of intuitions: Use of SNA (Social Network Analysis): Effect of common society and Government Organizations are continuously recognized as authority by exchange of innovation. The foundations are considered as the administrators of spreading new advances. SNA has been utilized to tackle an extensive variety of issues in Sociology and Anthropology (Kossinets and Watts, 2006). Studies are additionally found in the Economics writing, for example, contemplates on effect of systems on the selection of developments (Bandiera and Rasul 2006; Temel et al., 2003) adjustment to instabilities (Beuchelt and Fischer, 2006) and accomplishment in finding an occupation (Granovetter, 1973).

Use of SNA has as of late been made with regards to Agricultural Knowledge and Information System (Spielman et al., 2009) that conceptualizes rural learning improvement as the result of connection among numerous partners. This has additionally been connected for understanding Agricultural Innovation Systems (AIS) of the Third World nations (Spielman et al., 2009, Asres, Sölkner, Puskur, and Wurzinger, 2012). This application now should be extended for job framework examination, of which AKIS and AIS are parts. Sadly, this has once in a while been utilized as a part of the examination of rustic vocations, in spite of the fact that cases might be found where organize investigations have tended to a piece of occupation framework (Cinner and Bodin, 2010).

The network analysis will help us comprehend the individual and institutional systems that support rustic occupations, which lay ground for key correspondence and advancement intercession. Also, the initial phase in building limit with regards to systems administration in rustic groups begins from helping the provincial individuals and their specialist co-ops comprehend and imagine their current systems (Douthwaite et al., 2006). Truly, one of the survival techniques of the country poor, for example, negligible or little agriculturists, tenant farmers and landless workers, is their potential and capacity to get assembled and go about as a class with a specific end goal to satisfy their requirements or requests. On many issues, especially the ones which are of aggregate intrigue or which require haggling with the individuals who have power and expert, activation as a class assumes a key part as an issue of their technique. Once more, in course of their day by day life, circumstances regularly emerge when a need is confronted by a family which it needs to satisfy quickly even by taking assistance from others. In such conditions they act independently as a family unit or a family. They connect with each other as neighbors, companions, families, managers/representatives, and so forth. Consequently they step by step develop systems of customary communication through these ties (Jana and Choudhuri, 2013). We mark these systems as informal communities. These informal organizations work at family/family level and assume an essential part as a sort of procedure for survival of the rustic poor. Since one who has a place with such an interpersonal organization can ask for others in a similar system for help and support. Such streams of help and support work, in an unnoticed way, so to state, either

specifically, match shrewd, or through middle people in the system. Subsequently this procedure works underneath the surface, staying under the radar, yet relentlessly, to meet different dire prerequisites of day by day life and living that one can't satisfy by one's own particular assets within reach. Informal organizations, in this sense, give a procedure of asset assembly separately from those with whom one has arranged associations. Seeing such systems are of gigantic significance for genius poor innovative work.

A livelihood framework of institutions contains abilities, resources and exercises required for methods for living (Chambers and Conway, 1992). A reasonable job permits to adapt to and to recoup from stress and stuns, to keep up or upgrade its abilities and advantages for give feasible occupation chances to the people to come. A family unit's benefits comprise of the supply of assets used to create prosperity (Rakodi, 1999). Resources incorporate human capital (age, instruction and preparing, and family structure); normal capital (e.g., climate, water and land); physical capital (gear, domesticated animals, and power); money related resources (credit); area particular elements, (for example, access to framework and social administrations), and social, political, and institutional resources, including social and political systems, and social consideration.

A role based framework is a method for seeing how family units determine their role. A simple mind-set inside a farming system is utilizing the family triangle of benefits, capacities and exercises. Family unit individuals utilize their abilities and resources for complete exercises for maintaining employments. Family unit resources allude to the assets that families possess or have admittance to for picking up an occupation.

Role of Extension Workers and Institutions in 'Technology Transfer': The "Technology Transfers" is really an auxiliary procedure of learning. The key segments of an exchange can be distinguished as information, gets from true experience together with human skill fit for changing that learning energetically. Innovation exchanges incorporate a scope of formal and casual participation between innovation engineer and innovation searchers. Also, innovations exchanges include the exchange of information and specialized know how and additionally physical gadgets and gear (Atalb, Felipik and

Skowron, 2015). Chitambar (2015) characterized 'Social Organization' as the classes of human relationship structures wherein people deliberately related in efficiently coordinated units to progress and fulfil some ordinary purposes or interests that are not especially conveyed in the foundation. In affiliation each part has a formal status and part. It may be described as a social event with exceptional concern and interests that have developed a structure including specific parts for various people, and that have a practically formal course of action of rules and headings for operation. An affiliation differs from a foundation by its consideration on a scarcely confined reason. It is social event of people dealt with to look for after specific objectives. Affiliation may work inside association. Be that as it may, the idea of "establishment" is very extraordinary. Horton (1964) opined that foundation is a sorted out course of action of social associations which encapsulates certain consistent qualities and methodologies and meets certain basic needs of society.

Atalb, Felipik and Skowron (2015) opined that- after the exchange of rural innovations (agrarian innovation) to ranchers, which depends on their requirements for those strategies, it ends up plainly important to persuade them to embrace these new horticultural systems. It is the obligation of individuals working in the horticultural augmentation to induce ranchers to grasp the new innovation and agrarian innovation forms. The reception is a mental procedure which comprises of a few phases and identifies with the agriculturist's choice to acknowledge or dismiss a specific method.

Extension workers are work force who is in charge of meeting the objectives of augmentation framework. Notwithstanding, there have been less information on the parts and execution of augmentation specialists in the nation, despite the fact that there are sporadic reviews on feedback that expansion was not having the capacity to play out the fundamental changes in the country group (Sallam and Akram, 2005). As per Van lair Ban and Hawkins (1996) horticulture expansion is an open administration for HRD of specialists in agribusiness part, including agriculturists. In any case, the capacity of farming expansion is not just observed as vehicle for spreading logical and

specialized advance and innovation exchange. The horticultural expansion, in this manner, is a more extensive idea which stressed usage of undertakings, conveyance of learning and data.

The framework is likewise a road for shared association and opportunity that help individuals to create answers for their issues.

Mode of communication in family farms: Allwood (1985) in his article, the meaning of intercultural communication, possible problems between communication patterns problems and consequences related to intercultural communication were discussed in detail. Hossain, Crouch, Chamala (1992) described the mode of intercultural communication. This review explores the correspondence channels through which data on two rural practices is spread in a remote territory of Bangladesh. Two noteworthy cultivating hones, high-yielding assortments (HYV) of rice development and treatment of debilitated cows, were analyzed. The data looking for example on account of HYV development was described by an extensive number of supposition pioneers being accessible for counsels with other learned agriculturists outside the specimen towns, and by a multi-step relational correspondence design. On account of debilitated dairy cattle treatment, just three nearby conventional veterinary specialists were distinguished as key assessment pioneers. Not at all like HYV rice development, was the correspondence procedure in the treatment of debilitated steers immediate. The potential value of indigenous-based, fitting, appropriate, and adequate innovation is additionally delineated.

Mulvaney (1994) concentrated the valuable and suitable perspective of sexual orientation correspondence as a type of intercultural correspondence. He offers a short introduction on sexual orientation contrasts in correspondence with essential accentuation on cases that show how sex is both an impact on and a result of correspondence. To put it plainly, this dialog highlights essential pretended by correspondence in sexual orientation issues. Gillett (1997) in his study on the intercultural communication, Andy Gillett identify five broad areas which are- cultural behaviour: people from different cultures do things in different ways, students perceptions, culture, cross cultural pragmatics and language. On the other hand Jha and Chauhan (1999) described the intercultural communication issues. The principle components of this review were to look at the relational correspondence conduct of dairy ranchers in the Darbhanga area of Bihar. When all is said in done, it was found that age, arrive holding, crowd estimate and financial status were straightforwardly identified with the relational correspondence conduct of these agriculturists, though social interest and family size or sort had no such relationship. In their article, Fell (2000) depicted another improvement in correspondence hypothesis emerging from subjective science is quickly checked on as a reason for recommending that the utilization of words is a specific sort of activity with inconspicuous and significant outcomes that are effortlessly thought little of. This new intellectual science bolsters a changing rationality and style of farming augmentation that inclines more towards helpful learning. Certain examples of word utilization that happen in organized rural augmentation (orders and authoritative opinion, specialized language, holing up behind convention, exhaust words, feedback, arranging phrasing and parenthood articulations) are presented as boundaries to viable correspondence. Expanding dependence on email and the World Wide Web has conceivable advantages related with a more casual and by and by mindful utilization of dialect. Sinha and Sinha (2001) examine informal communication among rural women on home improvement in Haryana, India. Its specific objectives are: to find out the perceived importance of different home improvement message; to find out the informal communication pattern among rural women; and to study the places of informal communication in a village setting. Informal communication plays important role in transmitting innovative messages on home improvement.

Gasperini and Zulberti (2002) opined that 70 per cent of the poor live in rural areas. Despite the fact that education is a basic right in itself and an essential prerequisite for reducing poverty, improving the living conditions of rural people and building a food-secure world, children's access to education in rural areas is still much lower than in urban areas, adult illiteracy is much higher and the quality of education is poorer. In this regard, the Sustainable Development Department of FAO and UNESCO have joined forces to establish a new flagship on Education for rural people (ERP) within the Education for All initiative. The flagship seeks to address rural-urban disparities, which are a serious concern to governments and the international community as a whole. Le Baron (2003) inferred that each of the factors examined in this module - time and space, moral duty and destiny, face and face-sparing and nonverbal

correspondence are significantly more perplexing than it is conceivable to pass on. Each of them impacts the course of correspondences, and can be in charge of contention or the acceleration of contention when it prompts miscommunication or distortion. A socially familiar way to deal with struggle implies working extra minutes to comprehend these and different ways correspondence shifts crosswise over societies, and applying these understandings keeping in mind the end goal to improve connections crosswise over contrasts.

Singh, Narwal and Malik (2003) assessed the communication skills of 85 horticultural development officers (HDOs) working in the State Department of Horticulture, Haryana, India. Three broad areas of communication were considered: communication ability, communication quality, and preparation and use of audio-visual aids. Majority of the HDOs (64.71%) possessed fair communication skills, while 20% and 15.29% possessed good and poor communication skills, respectively. Correlation analysis revealed that mass media exposure, communication pattern, credibility of information, and role performance had significant and positive relationships with the level of communication skills of the HDOs. On the other hand, Barman, Pradhan and Majumder described that the correspondence level of ranchers from exceptionally urbanized towns in Dakshin Dinajpur locale, West Bengal, India, was evaluated in light of an examination of causal variables of agro-economic and socio-personal nature. Of these causal variables, trimming force, occupation, per capita pay, instruction, house sort, and material ownership had a noteworthy commitment in portraying the ranchers' correspondence level. Jiang (2006) examines intercultural correspondence and its centrality to advanced education. The paper quickly talks about culture, subculture and the meeting of societies. It additionally gives a short study of advancements in intercultural correspondence look into. The creator contends that receiving inter-culturalism in light of the standards of correspondence and regard at the national and institutional levels is more urgent than only acing some intercultural skills or applying some intercultural correspondence models plot in intercultural correspondence speculations. An experimental study, done by Prathap and Ponnusamy (2006)- on the relative effectiveness of four mass media channels (radio, television, newspaper, and Internet) on knowledge gain was conducted among 144 rural women belonging to self-help groups of three villages in Tamil Nadu, India. The selected technology, rabbit farming, was developed into parallel messages and was delivered through these channels to assess the knowledge gain. All the respondents (100%) had gained "adequate" knowledge after exposure to television, newspaper and Internet, while 97% of those exposed to radio had gained adequate knowledge after exposure. Traditional Medias were found to have a slight edge over new media in terms of influencing knowledge gain. Television was found to be the most effective treatment, followed by newspaper, Internet and radio.

CONCLUSION

Data, benefit, item are basic segments of the Sustainable Livelihood structure, basic to bolster basic leadership and execution forms at each level. A Strategic Program in Support of Sustainable Livelihood with extension agents ought to plan to enhance linkages between procedures of arrangement outline and usage, and the manageability, efficiency and benefit of employment results. Interpersonal organization in support of with extension agents, in this way, has three capacities: 1) to encourage the trading of data by the poor vital for economical jobs; 2) to enhance correspondence inside and between the establishments in charge of settling on choices that influence job alternatives; and 3) to engage poor groups to take part in the basic leadership forms.

Enhanced data alone however is not adequate for enhanced basic leadership. Basic leadership is a political procedure and partner interest in basic leadership procedures is critically imperative. The Sustainable Livelihood approach is on a very basic level individuals focused and requests a point by point participatory evaluation of the qualities and data needs of target recipients and partners as an early action in program plan. This needs to connect with partners at all levels, advance two-path streams of data amongst them, and focus on the part of data in connection to various business resources.

Present approach stresses multi-sectoral coordinated effort and associations between government divisions, open and private segment, common society and global improvement offices and looks to expand on existing qualities and openings and to supplement and upgrade existing frameworks. Systems to enhance joint effort between partners through, for instance consistent gatherings, workshops and courses, and new announcing strategies are likely thus be more imperative than presenting new data innovations, which ought to, themselves try to upgrade and reinforce existing advances as opposed to supplant them.

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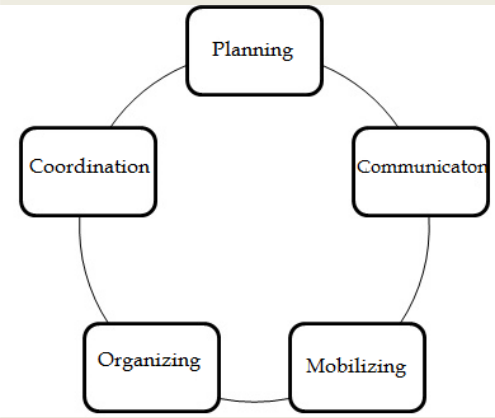
Exhibit 1

Professionalism and Development: Synthesis from review of literature

Many authors fabricated the roles and responsibilities of extension workers. The figure is the outcome of thorough review.



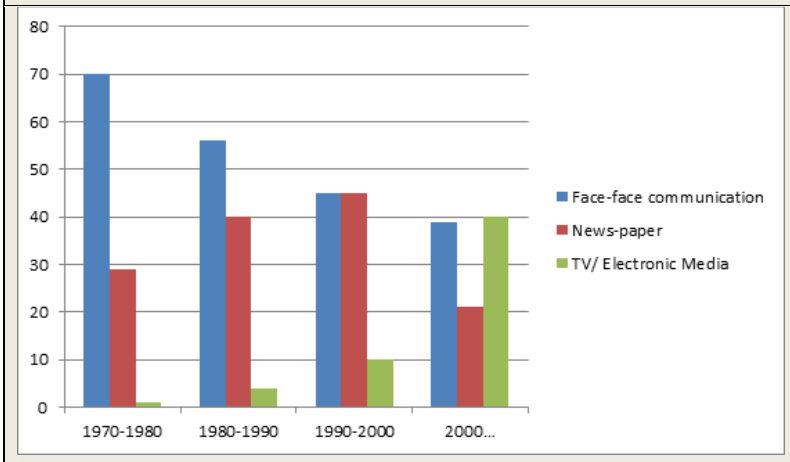
The extension specialists' part is to instruct the farmers about how to utilize new advancements. Information and use of expansion instruction standards, the augmentation labourers help a ton in deciding the necessities limitations, needs and open doors for farmers.

Figure: 1: Role of extension workers

Major review cited: Pretty and Chambers (1993), Carnea (1991), Bunch (1991), Aremu, , Kolo, Gana, Adelere (2015), Ann (2013), Chambers (1983)

Exhibit 2

Mode of communication in extension system



From the review of literature, it is clear that the use of electronic media has been increased in extension communication system since last decades.

Figure 2: Mode of communication: A glance from review of literature

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RESEARCH ARTICLE

Defining the Concept of 'Family Farming': Periphery and History

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ABSTRACT

Across the nation, traditional farm based livelihood system varied from the society to society, which curved the history of food self- sufficiency. In recent past, paradigm of farming system research has been shifted towards family based farming. Indian agriculture is not merely an occupation, but it is the way of life which for centuries has been shaped the life and out looks of the nation. It symbolizes peoples' struggle against economic deprivation. For centuries, tribes of this region have stayed in geographical isolation, have maintained their distinctive culture of farming, have sustained on subsistence family farms, and struggled to overcome poor socio-economic condition. Characterization of the farm resources and sustainability assessment of those farms are urgently needed, particularly in the context of natural resource management and socio-economic realities.

Keywords: Family Farm, FFS research, Evolution, Participatory Farm Analysis

INTRODUCTION

The idea of farming appears to be ingrained in this earth since 10,000 years. Since inception, Indian agriculture is not merely an occupation, but it is the way of life which for centuries has been shaped outlook of life and livelihood of the nation. For a considerable period of time, farmers of the developing countries have remained in topographical variation, have kept up their particular culture of farming, have managed on family based farming, and attempted to defeat poor financial condition. Agriculture all through the world is up 'til now single most basic human activity. Despite each one of the advances of so called 'development', it is so far the primary source of sustenance and a basic

origin of aspects and characteristic of society, whose produced substitutes are routinely not comparable to the normal components or all the more extravagant to make. The farming communities, throughout the third world countries, have remained outside the domain of the so called 'development' since they dwell in rural areas which are away from the cities.

There have, notwithstanding, been remarkable endeavors made by different reviews. According to World Bank (2008), Agriculture is a source of livelihoods for 5.5 billion people in the developing world of which 3 billion live in rural areas. Nearly 2.5 billion of these rural people are involved in agriculture of which 1.5 billion belong to smallholder households. These resource poor farmers constitute the majority (85%) of farmers in the developing world.

From the studies of eminent social workers and scholars like; Craswell (1998), Das (2013) it has been found that The concept of 'Family Farming' broadly refers to a special character of the farms which are sustained on the involvement of the family members with less dependence on high external inputs. Ever since the small farms depend on the family members and it created a tradition and culture of farming.

Triumph of the concept- 'Family based Agricultural System: During the end of 1950s, India faced a series of famine which shook the aspects of food security of the nation. This was a history of vulnerability and insecurity. Need for significant change in agricultural sector was felt. On set of 1960s, India launched Intensive Agricultural District Programme (IADP) to raise the food grain production. It was a significant developmental programme for the farming community which had been adopted, explored and evaluated. But it was not enough to ensure self-sufficiency in food production. At around the same decade Government of India launched a new programme, entitled as High Yielding Variety Prgramme (HYVP). It was a backup programme for Green Revolution. High yielding varieties, chemical fertilizers and input oriented approach created a vibration in the pulse of Indian agriculture. It was much more technical rather than institutional. Green revolution created a huge difference in Indian economy. But its impact was restricted in the periphery of the large farmers. Small and marginal farmers were unable to reap the benefits of this revolution. Rampant use of chemicals was ensuring the declination of soil health. As a matter of fact, it became an agenda of developmental priorities.

On the other hand, in our nation, greater part of the farming community has a place with small and marginal farmers (76.2%) who have just 29 per cent for operational holding, while 71 per cent of the worked region is controlled by farmers who have medium and expansive size possessions. The nourishment, feed and fuel generation should be expanded by 60 per cent in the following 25 years to address the issues of the developing countries. Hence, it is clear that majority of the farmers of this nation belong to small and marginal categories.

Thus a paradigm shift is advocated from high input based agriculture to the family based small farms which are embedded in the principles of productivity in perpetuity without associated ecological or social harm. The Green Revolution is shifted to the concept of an Evergreen Revolution when it is routed in the principles of ecology, economics, and social equity.

METHODOLOGICAL FRAMEWORK FOR REVIEW

Systematic reviews and meta-analyses are a key element of evidence-based literature, yet they remain in some ways mysterious. A review earns the adjective systematic if it is based on a clearly formulated question, identifies relevant studies, appraises their quality and summarizes the evidence by use of explicit methodology. It is the explicit and systematic approach that distinguishes systematic reviews from traditional reviews and commentaries. Whenever we use the term *review* in this paper it will mean a *systematic review*. Reviews should never be done in any other way (Med, 2003). Keeping in view the major thematic area and objectives, the review of literature was done.

Methodological Framework for Review of Literature consists of the following steps

- Fix the major area of work
- Determination of problem
- Search of literature
- Review of Context, Concept, Methodology, Theory and Evidences
- Analysis and interpretation
- Documentation

RESULT OF SYNTHESIS

Definition of Family Farming: Flashlight on the earlier research

From the studies of eminent social workers and scholars like; Craswell (1998), Das (2013) it has been found that The concept of 'Family Farming' broadly refers to a special character of the farms which are sustained on the involvement of the family members with less dependence on high external inputs. Ever since the small farms depend on the family members and it created a tradition and culture of farming.

From the studies of Das (2013), a researcher can get a clear line map of the context. On the last of 60s' when world was suffering from prolong and frequent hunger and food crisis. As we could no longer expand our production areas, the challenge was to increase the productivity to feed the fast growing population. The traditional agricultural systems were failing us. We needed to modernize our agriculture and we needed new technologies – as we were told. Green Revolution ushered in with the promise of giving us more food with promises of hiking up the productivity. It did so. World's food stores swelled over the next few decades. Whether that food reached our starved and half-starved countrymen, is a different story. Now, the modern technologies too seem to be failing us. Our rich agricultural crop diversity is wiped off, thanks to the handful of high yielding and improved crop varieties that now sway in our farmlands. Those who are left are threatened by GM crops. Rampant use of chemical fertilizers has led to the death of soil.

Hence, it can be concluded that it was the cause for which a paradigm shift is advocated for food production in the concept of low cost organic farming which is embedded in the principles of productivity in perpetuity without associated ecological or social harm. Side by side, farming system approach is now becoming prior concern. Collinson (2000) in his study cites FAO (1997): ''Farming System (FS) tries to look deeper into this crisis, particularly of the small family farms falling in between the modern and primitive production systems. The Farming System approach that evolved was based on the notion that: one had to begin with understanding the problems of farmers from the perspectives of farmers; and that solutions had to be based on a proper understanding of their objectives and their environments, including both biophysical and socioeconomic components''.

Comprehensive review of the past research studies is an essential component of any research endeavour, the major function of the review of literature is to get acquainted with various aspects of the term- 'Family Farming'. Some of the relevant studies which have been reviewed and analysed in line with theme of definition are given in logical order.

From the various articles it is clear that the definition of 'Family Farming' considers- 1) Labour utilization pattern in farm, 2) Family ownership of land over generations and 3) Farm integration with local community.

Bélièreset. al (2015) elucidates family farm as the ''forms of organisation of agricultural production and includes holdings that are characterised by organic links between the family and the production unit and by the mobilisation of family labour, excluding permanent employees. These links are reflected in the inclusion of the productive capital in the family assets and in the combination of domestic and market and non-market operating logics in processes to assign family labour and for its remuneration, as well as in choices for the distribution of products between final consumption, intermediate consumption, investments and accumulation''.

Aspects of the evolution of Family Farms

Illustrating this in respect to the history of family farming, Kesavan and Swaminathan (2014) cited an article, written by Hladik (2012). In that article he fabricated the complex procedure of food production at family farm and the way to serve the farm produces in family dining. Kesavan and Swaminathan (2014) also cited some chronological data, representing the emergence of family farms.

Mazyer and Roudart (2012) explained the history: if humankind somehow managed to permit each developed biological system of the planet to lie neglected, each would rapidly come back to a condition of nature near that in which it existed 10,000 years ago. Wild vegetation far more grounded than those current today would overpower developed plants and tamed creatures. Nine-tenths of the human populace would die in light of the fact that, in this Garden of Eden, basic predation (chasing, angling, and social occasion) would surely not sustain more than 500 million individuals. In the event that such a "natural calamity" was to happen, industry would be of little help, since it is not yet in a position to integrate nourishment for mankind on a huge scale, and won't have the capacity to do as such rapidly. Alongside these literatures, however, interpretation was made to analyse the history of the family farms.

CONCLUSION

Sustainability is essentially a social construct which can be interpreted in different ways by various groups in society. Ultimately, the components of managed ecosystems like farms need to function in such a way that productivity is maintained or enhanced over the long-term without the depletion of the natural resources (Scot et al, 2000). Daly (1973) had listed few general principles of sustainable development. According to him the main principle was to limit the human scale to a level, which is within the carrying capacity of the environment. Secondly, technological progress should be throughout efficiency measuring rather than throughout quantity increasing. Renewable resources should be exploited at a profit maximizing sustainable yield basis and in general not be driven to extinction, was the third principle. Lastly, for non-renewable resources, rate of depletion should not exceed rate of creation of renewable substitutes. Besides these market failure related to resource pricing and property rights should be created. Peet (1992) suggested that economic imperialism, ecological reductionism, and the economy as a steady state subsystem are three reasonably well-known strategies for integrating economics and ecology in the context of policy making in field of sustainable development. It reflects the biophysical system view of ecosystem as self-contained dose system needing only energy from the sun to produce the material requirement of the economy. A policy of sustainable development should be like one that seeks to promote efficiency.

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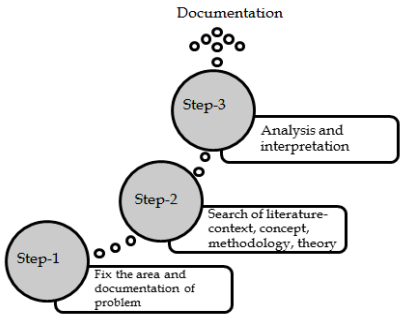

Figure1:Methodological framework for Review of Literature

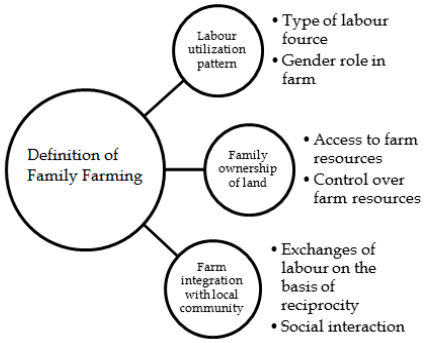

Figure 2:Definition of 'Family Farming': Analysis from review of literature

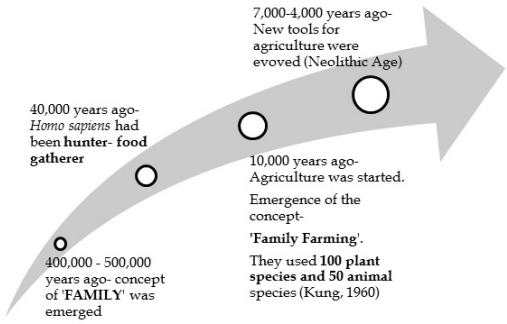

Figure 3:Emergence of 'Family Farming': A review based timeline

Table 1: Review based list: Definition of 'Family Farming'

Sl. No.	Source	Year	Title	Author	Key Concept
1	Food and Fertilizer technology -Centre for the Asian and Pacific	1998	Sustainable crop and soil management on sloping lands	Craswell, E.T.	Role of family members, Less external input
2	LEISA India, Bulletin No. 4,Vol.15	2013	Integrated Farming: An approach to boost up family farming	Das, A	Less external input, Labour utilization pattern
3	FAO's Family Farming website-http://www.fao.org/family-farming-2014/home/what-is-family-farming/en/	2014	Demands of Family Farming Organisations during the International Year of Family Farming IYFF-2014	FAO	Family structure, internal dynamics of family, gender role, farm resources
4	Current Science, Vol. 107, No. 12	2014	2014 International Year of Family Farming: a boost to evergreen revolution	Kesavan, P.C and Swaminathan, M.S.	Small holder farmers, policy support, mass production
5	International Land Qualition	2015	Women and family farming	Daley, E., Pallas, S. and Cangelosi, E.	Land management, family and community members, farm resources, natural resources

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RESEARCH ARTICLE

Gender Dynamics in Family Farms: Cases from Tribal Villages of East Singhbhum, Jharkhand

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ABSTRACT

For centuries, tribes of Chotanagpur plateau region have stayed in geographical isolation, have maintained their distinctive culture of farming, have sustained on subsistence family farms, and struggled to overcome poor socio-economic condition.This study highlights the family farms of tribal farmers in East Singhbhum district of Jharkhand.The study also considered the gender based productive dimension in farms. Productive dimension involves major activities like; Land Preparation, Seed Cleaning, Sowing and Transplanting, Intercultural Operation, Harvesting, Post Harvesting, Cattle Management, Milking. Keeping aside the aspects of the research problem, the perspectives of the methodology were inferred and identified. The research was construct chiefly with respect to Ex-post facto explore outline. As needs be, after an exhaustive and important detailing of the issues, particular targets were chosen. In the light of these goals, an exertion was made to make a careful audit of the applicable writing identifying with the past inquiries about in this field. Targets were given in the presentation part. This study is an amalgamation of descriptive research, correlational study and exploratory research.Finally, the study suggests some measure related to the problems and constraints of family farms.

Key words: Family Farm, Participatory Research, Participatory Rural Appraisal, FGD, Case Study, Jharkhand, Gender Dynamics.

INTRODUCTION

Work division of women and men in a farm fundamentally rotate around land and related assets. Notwithstanding these exercises each family unit requires the execution of a base measure of housework for carrying on its day to day exercises. The family unit constitutes a fundamental unit of creation in all such social orders where agrarian generation depends completely on utilization of family work (Sethi, 1991). The engrossment of farm members in farm based actions which are often discussed under the light of gender dominated domain undoubtedly discusses the role of counter gender. In a family based farm, the role of farm dwellers varies with their gender. But usually women are considered as the passive resources for the farm. As a matter of fact, it is not true. Women are the integral part of a Family based Farm. Over the last two decades, research articles explored the role of gender in farm activities. Goswami and Borodoloi (2013) described the situation as indicated by the NSSO information, in 2004-05, in country regions around 83 percent farm women were occupied with horticulture, either as cultivators or as workers, when contrasted with 63 percent of male farmers. Despite the fact that a huge extent of the rustic labourers is occupied with horticulture, yet they can get work for just a couple of months of the year.

Beyond the household activities, gender role in agriculture sector was highlighted by Singh (1980). He conducted his study at Panjab, India. He illustrated the role of women in agriculture: female interest in monetary action in the rustic ranges in the Punjab is firmly associated with land possession. Landowning individuals in the Punjab despite the fact that they claim little parcels, consider it underneath their poise to enable their ladies to work outside the home. They wouldn't fret ladies taking a shot at their own homesteads however they don't endorse working in the ranches of others. Creator presumed that there is nearly more financial improvement in Punjab however this advancement appears to be somewhat cut sided. Inside farming there is more prominent weight on sustenance grains than on business crops, in light of this there are not really any agro-based ventures in country ranges where ladies can take an interest in more numbers.

Rueben (1977) in his article, explained the extent of gender role, faced problems faced by the women in agriculture etc. were highlighted. Along with this, he propounded a framework equipped for representing the female's wage rate, male's wage rate and the nearness of kids as factors that decide the designation of time as between relaxation, home generation and market work. Samrit et al (1991) conducted a study at Bhadra district of Maharashtra. This study investigates the gender dimension vis-à-vis role of women in farms. Some major farming practices, preparation of organic manures and treatment of sick cattle, maintaining nursery, transplanting, were examined. It was found that these types of farm activities were extensively done by the women farmers. The study was conducted at the villages of Assam. The main factor of this study was to examine the role of women in paddy cultivation. In general, it was found that age, land-holding, herd size and socioeconomic status were directly related to the gender role in farms, whereas family size or type had most significant relationship (Siddiqui and Pathak, 1991). Hajiloo et al. (2007) esteem the part of rural women facilitators in enhancing the cooperation of provincial women and attest that rural women facilitators are pioneers who have solid communication with other women in the town and connection indigenous information with present day learning. Provincial ladies facilitators' fundamental part is in limit working for enhancing rustic ladies cooperation and confidence. Rimavi (2011) revealed that support of rural women who are the head of family unit is not as much as female from male-headed families. In addition, there is a noteworthy connection between ranch estimate and rural women investment in extension services.

METHODOLOGY

This study is an amalgamation of descriptive research, correlational study and exploratory research.This study is a blending of structured and unstructured approach.

Sample size: 270 samples were drawn by using Multistage Purposive Sampling.

Sampling Design: From the district, 3 blocks having >60% tribal population had been selected. Thereafter, 3 villages were selected from each block. After that, 30 farmers were selected from each village.

Selection of the study area

4. **Selection of the district:** Jharkhand is comprised of 27 districts. Out of this one district namely East Singhbhum was conveniently selected for the present study.
5. **Selection of the block:** There are 11 blocks in Deoghar district. Out of these 11 blocks, three blocks namely Ghatshila, Patamda and Baharagora block were purposively selected for the study.
6. **Selection of village:** Darisai, Bodhpur and Bhamradih villages of Ghatshila block, Dongagarh, Dhatkidih and Loraidoongri villages of Patamda block, Jarabani, Pochakhuli and Satpati villages of Bharagora block were selected.

RESULTS AND DISCUSSION

The gender influence in determining farm sustainability has not only been integral part but in recent past, it is the prior concern of farming research. To synthesize the gender role in agriculture, present researcher adopted 'Harvard Analytical Framework' (1985).

The 'Harvard Analytical Framework' is a network (otherwise called a 'matrix') for gathering information at the smaller scale level (i.e., at the group and family unit level). It is a helpful method for sorting out data and can be adjusted to numerous situations. The Harvard Analytical Framework has four primary segments (March, Smyth and Mukhopadhyay, 2005). They also expressed the feature of the instrument: This instrument recognizes all pertinent profitable and conception undertakings and answers the question: who does what?

Table 1 summarizes gender role in Family Farm. By using 'Stone Weightage' method, sex wise farm job distribution had been tried to understand. In this method, each of the respondents was asked to provide points against each combination of activity (Age/ Sex vs. Activity). The points should be given out of hundred. To make the procedure easy, hundred stones were used. After that, points were converted into percentage and ratio.

Productive Dimension involves major activities like; Land Preparation, Seed Cleaning, Sowing and Transplanting, Intercultural Operation, Harvesting, Post Harvesting, Cattle Management, Milking. It is noted that women involvement was equal in Sowing and Transplanting, Harvesting and Post Harvesting activities. Therefore, it can be inferred that Agricultural activities are both male and female centric, while allied activities are female centric. Along with this, gender role in reproductive dimension is also represented here.

Gender based access and control profile of Family Farms

Collected data describes the connection to gender based access to various resources of the family farms. The researcher used 'Harvard Tool' to analyse the gender role in family farms which is presented through the table underneath.

It is important to inspect which men and which women had access and control, and to ask what was really implied by get to and control for each case. (March, Smyth and Mukhopadhyay, 2005). Such inquiries for this research work would uncover the accompanying subtle elements.

Comments on the findings

Women of the study area marked significant influences and contribution to produce various crops. In the study area, they were involved in crop production, up to 60% of main crops for both the family consumption and market sale. The female candidates of the farms had access to land and crops, but rather the consequence of no control over input and market information. However, women had minimal access to the crop production and yield, while the control over these resources was made certain by male counterparts. In kitchen gardens, farm women were involved in vegetable productions that were essential to ensure food security. Farm women used to take part in nursery

management and harvesting. Women and their access on seed, market and land advances were likewise influenced by the people/ gender that had control and eventually possessed the yield. It is clear from FGD that men had access and control over seed, market and land. Female candidates of the families used to look after the animals. As discussed earlier, most of the reproductive activities like- Cow shed cleaning, Preparation of feed, providing water, poultry shed cleaning, collection of eggs and sale of products to neighbours were done by female members of the farms. Even though all male members of the families were not too much involved in livestock management, gender discrimination was prevailing in the decision making process regarding selling of those animals. Hence; it was found from discussion that the control over livestock was also secured by the male dwellers of the farm families.

Female dwellers of family farms were restricted to take decisions regarding off farm and community participation related issues. Almost in all walks of life, all over the place, women had prior responsibilities regarding household maintenance. Gender dynamics were prominently observed in this issue. Though women had access on the house hold and off farm facets, they did not have any access on those resources. While extension service related facets were controlled and accessed by the male and female both. It was happening because of the impact of mass sensitization which was ensured by several institutions working in the study area.

Gender based power-resource inclusion in extension services

Zimmermann and Maennling (2007) propounded this method to analyze the gender based resource insclusion in extension services. There was a boundless view that in execution arranged associations, honest to goodness power was alloted exclusively on the premise of mastery or authority abilities; in any case, this conviction was incorrect. In all institutions and extension agencies, power and control were manipulated in ways which were particular to the institution; they might likewise be legitimized by social institutions. People's own particular declarations about the premise of their position of energy were regularly enlightening and might incorporate cause, gender role and dynamics, age, property, impact, experience, learning, social and commonsense abilities.

In a family farm, male and female were acted as the major actors to ensure the allocation of power resource allocation. Figure 2 reveals the power-resource allocation pattern in extension services in terms of gender dynamics.

Comments on the findings

IN- Information

As because- male counterpart of the family had more control over the sources of information, content and information flow, hence; they had more influence on information dissemination. According to Zimmermann and Maennling (2007), power often derives from the control of information. Thus; it was clear from the result that male members of the families had more power which ensured better inclusion of information (from their part) in extension service system.

CN- Communication and negotiating power

According to Zimmermann and Maennling (2007), the basic facet of CN is- the ability to get a handle on the core of the issue and to impart unmistakably and briefly, passing on an intelligent message, inducing others and accordingly declaring one's own advantages. The study revealed that male member of family based farmers were able to grasp an information better than their counter parts. As they had more power to control and access the information sources, hence; they could convey the message easily. While female members had less power to control the information resurces which hindered the process of communication and nigotiating power.

KE- Specialist knowledge and expertise

Male dwellers of the family farms had more exposure and mobility. They had a societal power to dominate. It resulted to create a situation where they could avail more specialized knowledge and expertise rather than the women members of the family. As a matter of fact, women were unable to possess more power on specialist knowledge and expertise.

PR- Practical relevence

According to Zimmermann and Maennling (2007), control that emerges from educated aptitudes and encounter and is communicated in the capacity to take care of handy issues and in this manner realize change.From the study it was found that female dwellers had better performance in regards to PR. Female dwellers of farms who got exposure/ skill development training from voluntary organizations, were able to solve the real life situation/ problem.

CR- Creativity

Practical relelevance created vibration in the mode of expression. Hence; female respondents performed better in regards to employ facts in such a way that they were able to fabricate new thoughts and solutions. Hence, they had a better performance in this regards. Zimmermann and Maennling (2007) defined the fact: Control and power emerging from the capacity and aptitudes to use information and involvement such that they produce new thoughts, ideas and arrangements and give an inventive perspective of existing frameworks.

SR- Social Relationship

Zimmermann and Maennling (2007) defined: SR is the power which got from involvement of a social group, class, peer group and so on and defended by relations with different partners. From the study it was found that male dwellers had better performance in regards to SR. Male dwellers of farms had more exposure and mobility. Control and access to social groups generated a power of social relationship which had a clear influence on their farm.

Gender role in decision making

Without dynamic support of women and consolidation of female points of view at all levels of basic leadership, the objectives of equal improvement and peace can't be accomplished (Karl, 1995). Several reviews revealed that so as to build the part of female dwellers of farms in decision making for agriculture and allied sectors, it is important to document the gender role in farm decision making.

Ranking method of PRA was adopted to realize the gender role in decision making. It compares various criterions, based on gender role. The participants of PRA provided their choice against each criterion based on the discussion with other community members.

Major steps in the course of making 'the multiple ranking methods' encompassed of:

- Segregation of participants according to their Family Farm type
- Identification of the major farm and non-farm activities
- FGD on gender role.
- Preparation of matrix table.
- Voting against each criterion (by the participants).
- Collection of data from each village.
- Preparation of 'Cumulative table' for each type of Family farm.
- Analysing the responsible factors.

Table 3 were the outputs of PRA exercise. These tables provide a visualization of gender role in farm related decision making. However, raw tables of village level PRA data are not presented here. These tables are the 'Cumulative Tables', prepared on the basis of raw data.

It was revealed that farm women had taken part in various sorts of farm related decisions; however in a few perspectives their rights to settle on farm related decision making were smothered by the predominance of men.

Women's involvement in decision making regarding farm related activities like - deciding area to be sown under different crops , selection of new crop variety, labour hiring, selling of agricultural products were quite low or nil. In case of Farming System II and V, there was weaker gender participation in regards to 'deciding area to be sown under different crops'. But in other cases, it was nil. Crop related decisions were strongly taken by the males. Women

adults were generally not involved in the decisions related to use of fertilizer, labour hiring, and borrowing money. They had strong opinion regarding selection of feeds of animal. But marketing of the animals/ animal products were not their responsibility. They did not get the power to express their opinions regarding this issue also.

Constraints experienced by the women in operationalizing the family farms

In spite of the fact that ladies are assuming an indispensable part in little scale horticulture, yet different elements are influencing country ladies contributions in family cultivating. The beneficial and conceptive parts of females in the public arena, named as "double day" parts, brings about a heavier workload for females than guys, in spite of the fact that this likewise relies on upon social class, age or ethnicity assemble (Peter, 2006). However, since inception women's role in agriculture and economy has often been underestimated, and their involvement in agriculture has been invisible. Women's wide range of domestic activities, vast extent of family care, and immense involvement in cultural activities often create a shadow over their involvement in agriculture. Hence, highlight on 'constraintsexperienced by the women in operationalizing the family farms'- is getting impetus in the context of farming, not only in family farming but also in common perspective of whole agriculture. Constraints faced by farm women in their involvement in family farming were identified and presented in Fig 3.

Problem Tree is a type of diagram, mostly deals with cause-effect relationship of a problem. Constraints faced by the women during farming, are represented visually by using an outline/sketch of a tree. Major constraints are depicted through the stems of the tree. While roots of the tree represent the causes/ factors responsible for the constraints.

Using brainstorm technique respondents/ participants addressed the major constraints (like; difficult to spend time for farm operation, less involvement in farm related decision making, poor skill and knowledge etc.). Thereafter, outline of a tree was drawn by the community members on the ground with a stick. After that, causes of the constraints were identified. Attached diagram is a replica of original one. From Figure 3 it is reflected that lack of training and less exposure were the factors responsible for the constraint, pointed as 'poor skill and knowledge'. While 'lack of self-reliance', 'male dominance', 'cultural norms' and 'illiteracy' were responsible for 'less involvement in farm related decision making'.

CONCLUSION

The study also considered the gender based productive dimension in farms. Productive dimension involves major activities like; Land Preparation, Seed Cleaning, Sowing and Transplanting, Intercultural Operation, Harvesting, Post Harvesting, Cattle Management, Milking. It is noted that women involvement was equal in Sowing and Transplanting, Harvesting and Post Harvesting activities. As because- male counterpart of the family had more control over the sources of information, content and information flow, hence; they had more influence on information dissemination and decision making.

To ensure women's role in decision making, access to the resources of family farms should be the basic concern. Along with this, their access to knowledge and farm related training programmes should be increased. The constrained introduction to data sources restricts the information of farm women about most recent improvements in farm enterprises. Farm women were not effectively included in the exercises of different associations which give data about the farm innovation and improvements, and the majority of the women didn't know of the formative plans implied for their improvement. Hence, their liaison with the institutions should be ensured. The extension professionals ought to tell the individuals from SHG the agriculture credit and crop insurance for the assurance of life, property and obligation. Government had begun different farmers' protection plans for the advantages of dwellers of farm families. These plans ought to be highlighted to them. It ought to appreciate change and strengthening of farm women through state of mind change, inclination advancement, social cognizance and asset era. The imperatives of strengthening ought to be maintained a strategic distance from viably by creating certainty, dispersal of information and choosing the need for empowering women. Just dissemination or dispensing of Government fund does not help poor. The officers ought to approach to guide them how to utilize the funds and

assets viably and ensure empowerment through SHG. Vocational training along with mass sensitization will go a long way in improving the status and participation of farm women in agriculture and allied sectors.

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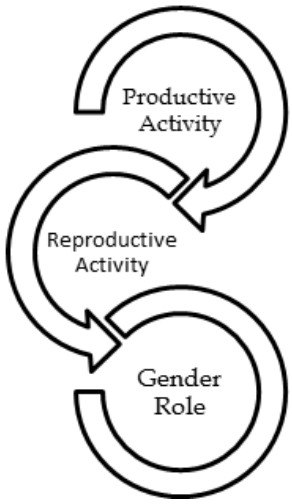

Figure 1: Gender activity in family farms: Harvard analytical framework

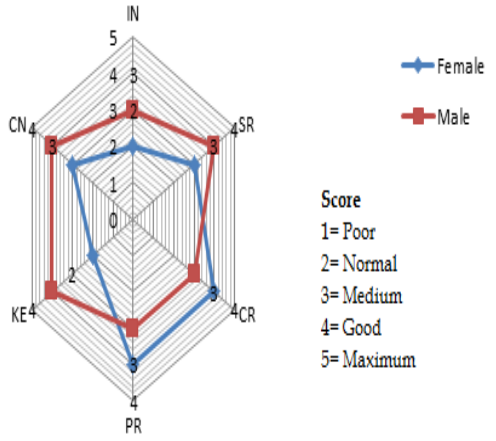

Figure 2: Gender based power-resource inclusion in extension services: Radar Diagram

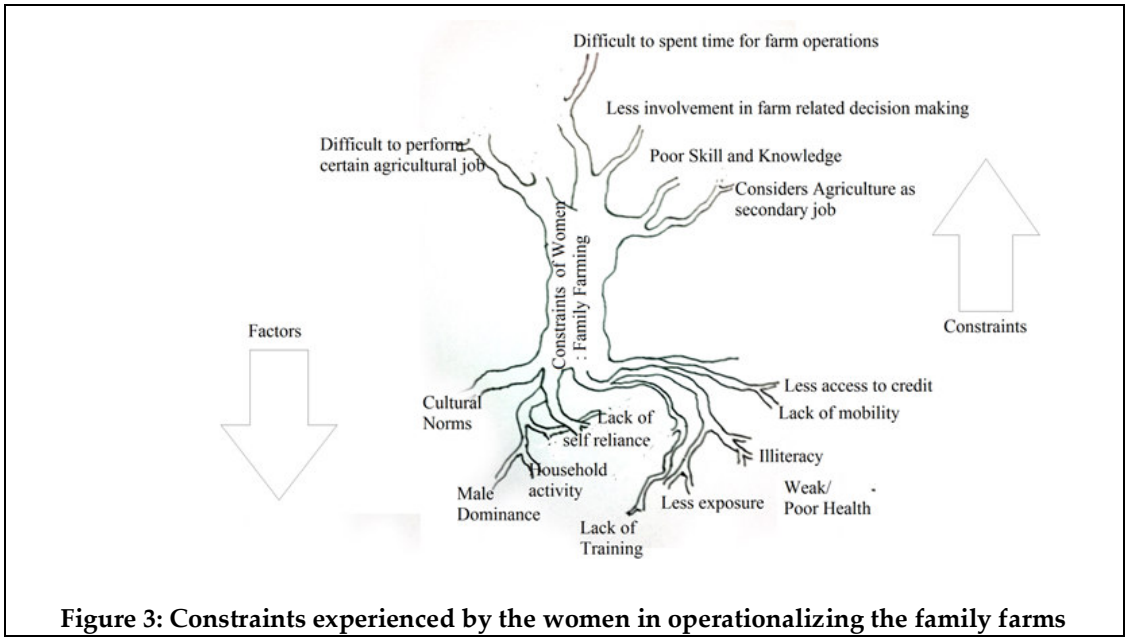

Figure 3: Constraints experienced by the women in operationalizing the family farms

Table 1: Gender division in farm related activities in Family Farm Type I
Production activities

	Male	Female	Both
Ploughing	✓		
Main field preparation	✓		
Nursery/ Kitchen Garden preparation			✓
Drainage	✓		
Irrigation (Main field)	✓		
Irrigation (homestead)		✓	
Sowing			✓
Weeding		✓	
Fertilizer application	✓		
Spraying	✓		
Harvesting			✓
Cleaning		✓	
Value addition		✓	
Market sale	✓		
Mulching		✓	
Sale to neighbour(Ag)		✓	

Reproduction activities			
	Male	**Female**	**Both**
Cow shed cleaning		✓	
Preparation of feed		✓	
Grazing of animals	✓		
Providing water		✓	
Sale to market(AH)	✓		
Sale of product to neighbour (AH)		✓	
Poultry shed clean		✓	
Poultry Feeding		✓	
Collection of egg		✓	
Sale to neighbour (Po)		✓	
Sale to market (Po)	✓		
Special care of birds		✓	
Buying fingerlings	-	-	-
After previous page….			
Reproduction activities			
	Male	**Female**	**Both**
Feeding fishes	-	-	-
Harvesting of fishes	-	-	-
Sale to market	-	-	-
Pruning/training	✓		
Thinning/gap filling			✓
Harvesting	✓		
Sale to neighbour		✓	
Sale to market	✓		
Goat shed cleaning		✓	
Care of goats		✓	
Feeding goats		✓	
Grazing of goats	✓		
Household Activities		✓	

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RESEARCH ARTICLE

Sacred Groves and Community Participation in Conservation of Natural Resources: A Case Study of 'Santal' Tribes of Palamu, Jharkhand

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ABSTRACT

The plateau of Jharkhand is not only popular because of abundance of mineral resources but also popular as it is the dwelling place of various tribes. Mainly 'Protoaustraloid' tribes are sprung from the earth of Jharkhand. They have their own lifestyle and culture. Their lives and livelihoods are mostly dependent upon nature and natural resources. There is a reciprocal relationship between nature and the tribes. Indigenous people still practice some cultural and ethnical linkages between social and biophysical ecosystem. Sacred groves are that kind of inextricable linkages between man and nature. Basically these are the tracts of virgin forests or the patches conserved by the local people for centuries and these are not merely a tradition but it is the way of life which for centuries has been shaped the relationship between man and its instinct to conserve the nature. The paper is the modest endeavor to highlight that the tradition of sacred groves could be an important tool to ensure natural resource conservation through community participation. The study was conducted with one of 29 groves of Palamu district of Jharkhand. *'Jaherthan'*s of the 'Santals' are selected as the groves. Qualitative approach has been adopted for the study. 'Participatory Rural Appraisal' is the integral part of this research work. The study was analyzed the management process with focusing on the utilization of biomass, source of conflict and it's resolution process, penalty process etc.and the lessons can be learned from such traditional initiatives in the broader context of the present policies related to natural resource conservation.

Keywords: Community Participation,Conservation, Jharkhand, , Natural resources, Sacred groves, Santal, Tribes.

INTRODUCTION

Since time immoral indigenous people are the protectors of the nature and natural resources. They have an unmediated relationship with nature. The traditional worship, ritual and practices symbolize the symbiotic relationship between these indigenous communities and nature. Indigenous people all over the world reside in harmony with the nature and conserved its valuable biodiversity.Seeland (1997) opines that human, for various needs, ranging from economic to belief system has utilized natural resources, which have been gradually integrated and incorporated in the social system of human beings by means of various institutional procedures. The economically developed world as well as some of the underdeveloped economies still depend on their own and the world's forest for survival, yet in different ways and meanings. Kala (2010) stated that the harmony between nature and human resource still exists. The indigenous people are still practicing their traditional culture linking with their social and biophysical ecosystem. Based on their traditional knowledge they maintain the diversity and productivity among the surrounding environmental condition. However, Khan, Khumbongmayun and Tripathi (2009) mean to ventilate that in course of time, science and innovation created and ventures were built up and extended to satisfy the expanding needs of the individuals. Different anthropogenic exercises have adjusted the structure and capacity of various environments everywhere throughout the world. One of the most prominent impacts of biological system annoyance has been the exhaustion of biodiversity. Vanishing of species because of natural surroundings adjustment, over exploitation, contamination, worldwide environmental change and intrusion of fascinating species is quick to such an extent that numerous significant taxa may evaporate even before they are recognized and their scientific worth is found. Indeed, even Kala (2007) raised his voice: The need of natural resources for human endurance had made them to advance a framework having some standard laws and practices, which in since quite a while ago run may assist with rationing the encompassing natural resources. Religion, being a ground-breaking instrument for persuading individuals, has consistently been utilized for meeting the ideal destinations of the society. The different righteous philosophies have contributed fundamentally in the protection of woods, biodiversity and scenes by proclaiming customary rules, practices and convictions. Be that as it may, with the appearance of business interests in the woods and biodiversity, in many parts of the world, the indigenous way of thinking and works on including righteous methodology received by the neighborhood networks for preservation of biodiversity have commonly neglected.

Jojo (2003) opined that after independence, capital intensive establishments were considered as *modern temples* of India. Baxi (2008) has been shown that no development without displacement became the *mantra* of developers everywhere. The tribal communities generally dependent on Forest- Hunting, Hill Cultivation, Plain Agriculture, Simple artisan and Folk Art etc. Due to urbanization, many of the tribal are migrating to different industrial belts and towns. Nature and natural resources are now treated as the 'Passive Resources'. It is because of industrialization, urbanization and its natural consequences. Expansion of urban areas and deforestation is goingg on parallely. Conservation and sustainable management of natural resources has become cef/ntral theme for almost all societies in order to meet shortages in timber or non-timber forest produce and overcome the impact of environmental pollution. Financial development in the midst of expanding ecological dangers will in general make a difficulty in numerous social orders which will undoubtedly develop in spite of the regularly restricted confinements of declining asset base (Seeland and Schmithusen, 2000). Numerous territories have been proclaimed as ensured regions and different in-situ and ex-situ preservation practices have additionally been attempted in various parts of the world. Numerous laws administering the biodiversity protection have additionally been authorized every once in a while including "The Biological Diversity Act 2002" ordered by the Govt. of India. Other than these proper laws, there were numerous customary preservation practices of indigenous societies in numerous segment of the world, which added to the preservation and assurance of biodiversity. A genuine case of such customary practices is the preservation and assurance of small woodland fixes by committing them to the neighborhood gods by different indigenous societies of the world. Such woods patches are designated "sacred groves" (Khan, Khumbongmayun and Tripathi, 2009).

These indigenous people utilize the natural resources of a given region over generations and quite expect that these resources would secure their future generation. This probably paved way emergence of different cultural institutions and rituals to ensure the sustainability of the natural resources. This may be the basic truth lies behind the emergence of 'Sacred Groves'. Sacred groves are that kind of inextricable linkages between man and nature. Basically these are the tracts of virgin forests or the patches conserved by the local people for centuries and these are not merely a tradition but it is the way of life which for centuries has been shaped the relationship between man and its instinct to conserve the nature.

Gaikwad, Paralikar, Chavan and Krishnan (2004) portrays Sacred Groves as a deep rooted convention where a fix of backwoods or water body is devoted to nearby divinities and none is permitted to slice plants or to massacre creatures or any type of life.

While Buchman (1992) highlights that that the tradition of sacred groves could be an important tool to ensure natural resource conservation: sacred grove contains a large number of species and is considered to be a true ecological jewel. This territory harbors an immense wealth of biological and genetic diversity and provides safety to endangered animal and plant species and probably constitutes only representation of forest in its virgin condition'.
The plateau of Jharkhand is not only popular because of abundance of mineral resources but also popular as it is the dwelling place of various tribes. Mainly 'Protoaustraloid' tribes are sprung from the earth of Chotanagpur plateau. They have their own ligfestyle and culture. Their lives and livelihoods were mostly dependent upon nature and natural resources. There was a reciprocal relationship between nature and the tribes. The paper is the modest endeavor to highlight that the tradition of sacred groves in Jharkhand could be an important tool to ensure natural resource conservation through community participation.

Objectives of the study

Keeping the aforesaid objectives in view and looking atthe tradition of sacred groves at Palamu district of Jharkhand, the study was conducted with some specific objective:
To understand the community's perception about the tradition and natural resource conservation
The empirical study was conducted with a broader objective: *Acquired lessons can be learned from such traditional initiatives in the broader context of the present policies related to natural resource conservation.*

Research design

The present study is a descriptive one. The study is also based on participation based Ex- post facto research design. Based on the research problems, specific objectives were decided. Basically based on review of literature, the problem and related issues were understood. After that, the process of data collection was started.

Locale of the study area: The present study was conducted at the picturesque hamlet ofGhanseeTola of Palalmu district of Jharkhand, India.

Sample size (n) of the study was 60 from 20Santal families, nearer to the Sacred Grove locations i.e. 3 from each family. The respondents were divided according to their age and sex (Middle aged male and female, Youth and Aged persons).In order to select the sample, purposive sampling was done.

The methods of data collection were qualitative in nature and were aimed to seek answers to certain research questions which would be deducted from various studies, researches and also during the field study. Given below is a list of the major techniques of data collection utilized by theResearcher-author for the present study:*Interview, Observation (Participant Observation and Non-Participant Observation), Focused Group Discussion (FGD) and Participatory Rural Appraisal (PRA).*

The findings of this study had been discussed after analysis of the collected data and were subsequently summarized. The conclusion and the suggestions were aiming to bring desired positive contribution to the natural resource management.

RESULT AND DISCUSSION

As a rule,Santals go around their nearby indigenous divinities. Santals arrange their righteous function at the hallowed place 'Jaherthan'. It is situated in the center of the woodland. It might be the border of the village.

A number (30-35) of Sal trees (*Shoriarobusta)* are the integral part of '*Jaherthan*'. Three trees are essential and they must be in a row. At the base of each of these three trees sacred stone is placed which symbolizes the deities Jaher era, Marang BuruTrukoand Muruko. Near those three Sal trees and a stone is put on an Asan tree**'s** base representing the deity ParganaBonga. There is also a Mahua tree (*Madhucaindica*); on its base, a stone representing the deity Gosain (Lady of the grove) era is present there.

The village dwellers themselves maintained the sacred groves with a great passion and sanctity. The traditional institu mechanisms have been helping the local people in maintaining the sacred place '*Jaherthan/ SarhuliMandir'*. The 'Jaher' has given the duty to the KudumNaike (priest) to oversee and prayer the village divinity in holy forests. There were a few traditions and social practices related with assortment and for the most part there was no limitation on the assortment of the products, anyway the nearby individuals feared assortment from the sacred forests. There was a general conviction that since holy forests were holy, the finders may be rebuffed by spirits and gods for unapproved assortment of natural resources, however all gods were not viewed as perilous.A c onviction was additionally connected with the old tree species that old trees in hallowed woods for the most part the frequent of malevolence spirits, and as old as the tree, more noteworthy the odds of shrewdness spirits to possess. The nearby individuals dreaded to go to such places, even in the early afternoon and evening. Youngsters and pregnant ladies were not permitted to visit such places. This kind of conviction assists with shielding from the everlasting greediness of individuals.

Seasonal Festival Calendar: Seasonal Festival Calendar, obtained from PRA, is redrawn here from the original to make it visible, as the hazy photo copy of the main sheet may not be properly understandable.

The calendar clearly depicts the festival seasonality. '*KudumNaike'* is the priest of the community. Annual Important rituals and Festivals showing their relation with Agricultural

It is commended to feel the delight of reaping crops. Pigs, eggs, fowls and goats are offered by the village Naeke (priest) in the Jaherthan (holy woods).

Baha is celebrated in the month of Feb.-March *(Phagun).* The first fruits of *Matkom(bassialatifolia)* and other wild fruits and flowers, mainly the S*arjom (shorearobusta)* flower arebeing offered. The N*aeke*and the K*udamnaeke*offer sacrifices of fowls at sacred grove in honourof *Maran Buru, Jaher Era* and *Moreko-Turuiko*.***Erok Sim*** is celebrated in the month of *Ashar*(June-July). Sowing of rice seeds in the field.The *naeke*sacrifices the fowls to the J*aherbonga*sand the M*anjhibonga*, invoking each one ofthem to make the earth fertile.***Hariar Sim*** is celebrated in the month of *San* (July-August). It is the time when the Paddyseeds start Sprouting. The *naeke*sacrifices fowls to the village *bongas*, namely *Maran Buru,Jaher Era, Gosae Era, and Moreko-Turuiko, Parganabonga, Manjhibonga*and *Simabongas*for a luxuriant growth of paddy. *Iri-GundliNawai*is celebrated in the month of *Bhador*(Sept.-Oct.). The first fruits of the millet*iri*(*panicummillaceum*) and *gundli*(*panicumfrumentaceum*) are offered to the *bongas*.The*kudamnaeke*along with the fruits of the millet offers sacrifices of goat or ram to the *parganabonga*to protect their crops from rats or other pestilence. *Jantharis celebrated in the month of Aghar*(Nov.-Dec.), the first fruits of the winter rice crop offering. The *kudamnaeke*offers sacrifice of goat or ram to the *parganabonga*along with the first ears of paddy to protect from stomach disease, to multiply the paddy and also to protect their grains from harm. ***Magh Sim*** is celebrated in the month of *Magh*(Jan.-Feb.), when the *sauri*(thatching grass) is being cut.Fowls are sacrificed by the *naeke*to the village *bongas*, invoking them to multiply their *sauri*crop.

Conservation of Nature: Myth of the Goddess of the Sacred Grove: The *JaherEra*is the Lady of the Sacred Grove (*jaherthan*) over which she presides. There is no idol of *Jaher Era*. She is considered to be the benevolent spirit who tends the other spirits at the *Jaherthan*and look after the interest of the village and never does any harm but is

mainly concerned with their bodily needs. She is usually worshiped at all festivals for the general welfare of the village, especially for obtaining good crops and for the health of the villagers and their cattle.

Sacred Grove Resource Map: It shows 'spatial dimensions' of natural resources available in the Sacred Grove. It is important to allow enough room (on the ground) to show common sources and plant diversities and some distance away from it. People may forget to show certain resources on the map, in which case it will need to be revised: thus, a copy of it should not be made until the discussion has been completed. The whole map was drawn by the respondents. The Sacred Grove Resource Map obtained from PRA, is redrawn here from the original to make it visible, as the hazy photo copy of the main sheet may not be properly understandable. The Map reveals:A number (30-35) of Sal trees (*Shoriarobusta)* are the integral part of '*Jaherthan*'.

Three trees are essential and they must be in a row. At the base of each of these three trees sacred stone is placed which symbolizes the deities Jaher era, Marang Buru Truko and Muruko. Near those three Sal trees and a stone is put on an Asan tree's base representing the deity ParganaBonga. There is also a Mahua tree (*Madhucaindica*); on its base, a stone representing the deity Gosain (Lady of the grove) era is present there.

Along with this, the Sacred Grove is the rich source of Ethno-Medicinal Plants like; Latapalas (*Butea superba*), Kalmegh (*Andrographispaniculata*), Bandar Lathi (*Cassia fistula*) etc.

Impact Chain/ Pathway (Community Perception): The Impact Chain/Pathwayis a flow diagram, commonly used to identify and depict the impact of an activity, intervention or event. Impact Diagram not only captures the planned changes, but also takes into account other types of changes as perceived by the local people. The impact can be positive and negative and planned or unplanned. In fact, the Impact Diagram made by the local people generally portrays effects that outsiders would never have been able to think of. Impact Diagram has been used for various purposes including:

1. Identification of impact, intended and unintended as well as positive or negative.
2. Understandings inter linkages between various effects.
3. Discussion of impact, leading to an understanding of reasons for change.
4. Planning how to control and minimize the negative impact.
5. Assessing the impact of various interventions.

This impact pathway will depict the impact of Sacred Grove on the local community.

The whole map was drawn by the respondents. The impact pathway of Sacred Grove, is redrawn here from the original to make it visible, as the hazy photo copy of the main sheet may not be properly understandable.

From this impact chain it can be opined that traditional rules often prohibit the felling of trees and the killing of animals, except in special cases do allow collection medicinal plants by local people (only through the *Naike*s)

Challenges to maintain the Sacred Grove: To get their perception about the challenges, faced by them to protect or maintain the tradition of the sacred groves, adoption of another PRA tool i.e. 'Problem Ranking throughMatrix Scoring method' was done.

Here people firstly selected the challenges, there after the ranking procedure started. The table shows, people realizes that the forest/ sacred grove is in danger and basic reasons behind this are: 1. Degradation of forest and 2. Lacuna in maintenance of the sacred groves. They pointed out that it is because of human activities. They claimed that urbanization has a huge impact on it. There after they pointed out a basic human instinct i.e. greediness. Like this way they analyze their own situation.

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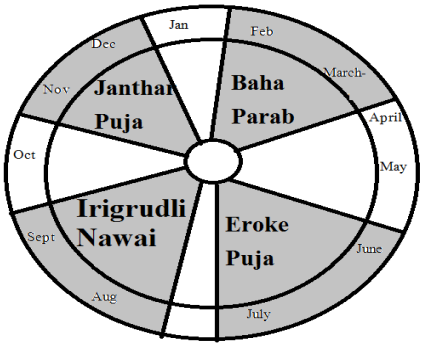

Fig:1.1 Seasonal Calendar

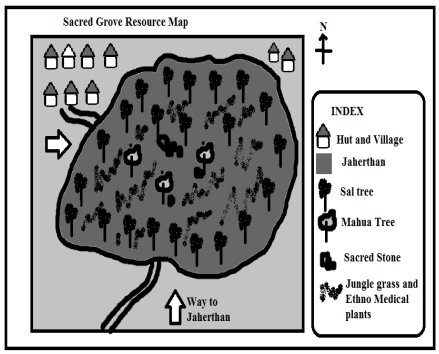

Figure 2: Sacred Grove Resource Map

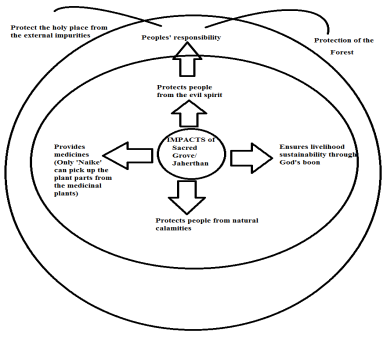

Figure 3: Impact Chain of the sacred

Table 1: List of the Ethno-Medicinal Plants (Prepared trough people participation)

Sl. No.	Species	Local Name	Plant Parts Used	Medicinal Value	No. of plants
1	*Butea superba*	Latapalas	Stem, bark,seed	Bark/gum cures piles; Useful as sedative and antihelmintic.	10
2	*Cassia fistula*	Bandar Lathi	Leaf, fruit, seed	Used in fungal infections, Urinary troubles	5
3	*Andrographispaniculata*	Kalmegh	Whole plant, leaf.	Cures dysentery, worm infection; Good for liver	12
4	*Jatropha. gossypifolia*	Bherenda	Shoot, leaf.	Used in dental diseases, carbuncles	10
5	*Ocimumcanum*	Bantulsi	Leaf	Used in skin diseases and cough and cold	6
6	*Vitexnegundo*	Nishinda	Leaf	Used as tonic, antiseptic, antihelmintic, tranquillizer.	4
7	*Aristolochia Indica*	Ishermul	Root, stem, leaf.	Used as tonic, stimulant; cures	7
8	*Curculigoorchiodes*	Talmuli	Rhizome	Used as appetizer; cures diseases of blood and leucoderma	12
9	*Croton bonplandianum*	Churchuri	Leaf.	Used as blood-coagulant, antiseptic	5
10	*Bauhinia vahlii*	Latakanchan	Root, bark, leaf, seed.	Used as aphrodisiac, tonic; cures dysentery	6

Table No2: Problem Ranking through Matrix scoring method

Activity	Degradation of Forest	Lacuna in Maintenance	Total Score	Over all Rank
Urbanization	7	8	15	1
Greed	6	8	14	2
Lack of dedicated man- power	4	7	11	3
Poverty	5	5	10	4

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RESEARCH ARTICLE

Women Empowerment through SHGS: Looming Lights from the Tribal Villages of Jharkhand

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ABSTRACT

'Women Empowerment' has been now an important phrase of discussion for the social scientists. The concept of 'Empowerment' was firstly highlighted by the Political Scientists. Undoubtedly, effective utilization of human potentials and realization of knowledge about him/herself are believed to be the most critical capabilities of individuals. Probably this is the root of 'Empowerment'. The term 'Women Empowerment' symbolizes women's realization about their potentials. On the other hand, SHG approach intends to highlight towards unfolding the potentials of women through group approach, enabling them to help themselves by their own capacity. In spite of this, the condition of women SHGs is in doldrums. This might be quite difficult to generalize the whole scenario. Not because the SHGs are not sustaining but because there are too many success stories, revealed according to various voluntary organizations. The study is a modest endeavor to revisit women SHGs (developed by NGOs) of Deoghar and East Singhbhum districts of Jharkhand. Of the various factors attributed to tribal socio-economic life, family based farming, important feature is gender role. Tribal women in almost all walks of life are sharing responsibilities in domestic as well as economic sector. The study is based on Ex- post facto research design. The methods of data collection were quantitative and qualitative in nature and were aimed to seek answers to certain research questions. Participatory Rural Appraisal and FGDare being the

dominant methods. Keeping a foreside to the main objectives, the study emphasizes on socio-economic, political, entrepreneurial aspects of empowerment. Finally, the study suggests some measure against the problems and constraints of the SHGs.

Key words: SHG, FGD, Women Empowerment, Participatory Rural Appraisal, Jharkhand, Gender Role.

INTRODUCTION

Women Empowerment: 'Women Empowerment' has been now an important phrase of discussion for the social scientists. The concept of 'Empowerment' was firstly highlighted by the Political Scientists. Undoubtedly, effective utilization of human potentials and realization of knowledge about him/herself are believed to be the most critical capabilities of individuals. Probably this is the root of 'Empowerment'. The term 'Women Empowerment' symbolizes women's realization about their potentials.

After independence all round efforts have been made to promote the welfare of the women. Article 15 of Constitution confers the equal rights of both sexes, though the state could make any special provisions for women (Kabeer, 1998). The introduction of English education and the contact with the western nations kindled the rationalistic spirit of the people (Mishra, 2006). Biju, (2006) opined that social differentiation & inequality are universal phenomenon.

According to World Bank, (2001)Since the 1990's women have been identified as key agents of sustainable development and women's equality and empowerment are seen as central to a more holistic approach.

'Feminism of Poverty': Not an illusion: In recent past there has been a trend to analyse poverty in the context of gender issues. The concept of 'Feminism of Poverty' critically linked poverty with women related issues. Now role of women varies from society to society. But 'Feminism of Poverty' often proves that women empowerment is one of the strong weapons to struggle against poverty. Let's check some statistics. A 1992 UN report disclosed that "the number of rural women living in poverty in the developing countries has increased by almost 50% over the past 20 years to an awesome 565 million -- 374 million of them in Asia, and 129 million in Sub-Saharan Africa. ... While poverty among rural men has increased over the last 20 years by 30%, among women it has increased by 48%".

Women in India contribute 89 per cent of the unrecognised sector and it is reality that their participation rate is higher in rural areas. Women responsible for one-third of the labour force of India and 90 per cent of the rural-urban women are unskilled workers. Hence, women empowerment could be a mechanism to pave the way for integrated development. Although, gender discrimination has been banned by the Constitution and women have been guaranteed political equality with men, yet there is a difference between the constitutional rights and the rights enjoyed in reality by women. Even after half a century of independence, barring a few exceptions, women have mostly remained outside the domain of power and political authority.

Bhuyan, (2006) highlighted the issue in different context. He opines that although they constitute about half of the citizen and over the years their participation by way of voting has increased, yet their participation and representation in law making and law implementing bodies are not very satisfactory. No doubt the 73rd and 74th constitutional amendment acts have provided access to women in the decision making process at the grass-root level but their representation in the Parliament and state legislatures is woefully poor. Insecurity does not allow the women leaders to identify leadership at the grass-root level. In politics when a man proposes, they themselves depose. In reality women representatives are ornamental in nature and political consciousness is found lacking among them. They are affected by the caste and class divisions, feudal attitudes, patriarchal nature of the family and village-social, environmental, ethnic, religious separatism and the like. They are members on record only. Allegedly, they are not consulted while taking decision. Thus, women representatives are not free from male dominance in the village administration and no significant change in the power equal is observed in the villages.

SHG: Concept and Context

Indhumati and Palanivelu (2013) stated that Self-Help Groups are increasingly accepted as agent by social changes, development and empowerment among the women. SHG's approach represents a paradigm shift from development toward empowerment. The SHG's are considered as the agents of transformation through the mobilization, organizations, banking in situation and voluntary organizations follow self-help approach to active rural development and empowerment of the women in India. The banking institutions channelize their credit to poor through the SHG's.

Self Help Groups are small homogeneous group of individual members who voluntarily come together and form an association for the purpose of solving their common problems through self-help and mutual help and for achieving a common objective. In most cases SHGs are constituted by persons known to one another and coming from the same village, community or neighbourhood, that is, SHGs are small in size with membership ranging from 10 to 20 are homogeneous (poor, financially weak, same socio-economic background etc.) and have certain pre groups binding factor. These groups start and promote with small saving in a common group-fund and kept in a bank. (Vadivoo and Sekar, 2004).

Research Objectives: With these rationales at the backdrop, the objectives for the study were –

- To analysewomen empowerment in the light of pre and post SHG situation
- To find out the role of institutions in women empowermentthrough SHG
- To trace out major constraints of the SHGs

METHODOLOGY

Research design: The study is based on Ex- post facto research design. The methods of data collection were both quantitative and qualitative in nature and were aimed to seek answers to certain research questions. Participatory Rural Appraisal and FGD are being the dominant methods. Keeping a foreside to the main objectives, the study emphasizes on socio-economic, political, entrepreneurial aspects of empowerment. Participatory approach is adopted to analyse the whole situation.

Locale of the study area: The study was conducted in the selected areas of Patamdablock of East Singhbhumdistrict andDevipur block of Deoghar, Jharkhand.

Sampling procedure: Multistage sampling technique was adopted for the selection of study area and sample respondents for collection of information required for the study.

RESULTS AND DISCUSSION

Women Empowerment: In the light of Pre and Post SHG situation

Social Empowerment: The present study intends to find out the social empowerment of the women, residing at Deoghar and East Singhbhum district on the basis of social empowerment indicators like employment selection freedom, decision making ability, social equity, employment skill, ability to defend themselves and ability to participate in social issues, autonomy in decision making.

Cobweb Diagram: It is a participation wheel, popularly known as evaluation wheel. The method deals with visual representation of perception of the masses to reveal the relative social status of SHG and Non-SHG members. Here 'Cob Web Diagram' has been utilized as an evaluation tool to measure the social empowerment of women in pre and post SHG situation. The empowerment issues were selected on the basis of pre-determined variables.

Firstly the purpose of the PRA exercise was explained. Then participants were requested to provide score against each of the five variables. They agreed to score each of the groups on the five indicators on a five point scale. Scores obtained from separate blocks of Jharkhand, had been transferred into a 'Cobweb Diagram'. Respondents of four blocks have been represented by the four quadrants. These four arms of the diagram are considered as four scales. Performance of each block has been marked using different symbols on the indicators.

The size of the trapezoid thus indicated the empowerment status of women of different blocks on the particular indicator. Thus, bigger the size of the symbolic line (indicator) symbolizes better social empowerment status of the women. Women performed well in skill of problem solving, social status, and selection of employment. Women of Patamda and Musabni (East Singhbhum) are more socially empowered in comparison to other blocks (Deoghar).

Economic Empowerment: Economic empowerment is the ability to access, own and control resources. It can be measured in a variety of ways, using outcome indicators such as income generation, ownership of assets and land, expenditure patterns, degree of participation in paid employment, division of domestic labour and control over financial decision-making.

In post SHG situation, the women respondents were able to meet up financial requirements of family like paying children's fee for school and private tutor, electric bill, medical expenses, household items etc. Some of them were even able to manage regular savings by deciding on priorities heads of expenses. Thus, at times of family need, they were able to contribute from the savings which improved their status and respect in families.

Impact on income: Income is one of the important indicators to investigate the level of living of the members of the society. The data regarding the average house-hold income of beneficiaries was estimated in two point time i.e. 'Pre' and 'Post' SHG situation. Table 2 shows the income of the SHG members before and after joining the SHGs.

Rank Test is applied to test the significance of difference between the annual incomes of SHG members before and after joining SHG in table above.

a. Based on negative ranks

b. Wilcoxon Signed Rank Test

Since the asymptotic significance value is less than 0.05, we reject the null hypothesis that the there is no difference in income before and after joining SHGs. The number negative ranks for Income after Joining SHG – Income before Joining SHG is given in the following table. It is trivial from the table that for all the respondents Income after Joining SHG is higher than Income before Joining SHG.

c. Annual Income Before = Annual Income After

Chi Square Test for Economic Empowerment

The respondents level of empowerment on the basis of their experience as members of the SHG analysed, among them 10 respondents had a low level of empowerment, 156 respondents had a medium level of empowerment and 14 respondents had a high level of empowerment. To evaluate the empowerment of women entrepreneur through Self Help Groups, chi-square test has been used.

The table value of χ^2 at 0.05 level of significance at 6 degrees of freedom was 13.67. As the observed χ^2 value i.e. 83. 67825 is greater than the table value i.e. 13.67, so it can be said that women were economically empowered through SHG. It revealed that the SHG had been successful in providing economic empowerment to their members.

Economic Empowerment in Post SHG situation: Cobweb Diagram: Here 'Cob Web Diagram' has been utilized as an evaluation tool to measure the social empowerment of women in pre and post SHG situation. The empowerment issues were selected on the basis of pre-determined variables.

Firstly the purpose of the PRA exercise was explained. Then participants were requested to provide score against each of the five variables. They agreed to score each of the groups on the five indicators on a five point scale. Scores obtained from separate blocks of Jharkhand, had been transferred into a 'Cobweb Diagram'. Respondents of four blocks have been represented by the four quadrants. These four arms of the diagram are considered as four scales. Performance of each block has been marked using different symbols on the indicators. The size of the trapezoid thus indicated the empowerment status of women of different blocks on the particular indicator. Thus, bigger the size of the symbolic line (indicator) symbolizes better economic empowerment status of the women. Women performed well in Self-financing and saving habit. Women of Patamda and Musabni (East Singhbhum) are more economically empowered in comparison to other blocks (Deoghar).

Psychological Empowerment : Psychological Empowerment involves a sense of autonomy, competence, efficacy, meaningfulness and trust.

Garret's Ranking : clearly depicts that self-employment is the main factor influencing the empowerment of women entrepreneurs through SHGs.

Major findings fromGarret's Ranking: The variable 'Self – Employment' obtained highest score .The least score is awarded to 'Serving the Society'. It is inferred that 'Social Status' and 'Group Domination' are the important factors for the SHG members.

Political Empowerment: Traditionally women were considered a passive worker in the society. Hence, political empowerment is needed to melt the ice. Political empowerment has direct relationship with social empowerment. This dimension considers the issues like- Political Awareness, Protest Power, and Participation in election and Panchayat meetings. Although many aspects have been considered, they do not cover all aspects of political empowerment. Moreover, due to variation in mental and socio-economic conditions, the aspects may vary from society to society. Leadership quality is now considered as the major aspect of political dimension.

After joining SHG, the members' level of awareness in political, educational and legal fields had increased. They were well informed about their local leaders and 25% of the respondents have some knowledge about the Nation's political affairs. Almost all the members even knew the legal age of marriage for boys and girls, dates of election as well as the nominated candidates. From the Figure 2, it is clear that the status of political empowerment became better in post SHG situation. 'Protest to Power' has increased significantly.

Role of institutions in women empowermentthrough SHG:

NGOs are sensitizingprimary stake holders (women) and they could play a significant role in initiating a SHG and also arranging technical skill development programmesfor the SHG members. Women are often able to impart technical knowledge and skill.Some NGOs are also trying to develop marketing chains in the process of establishing on an enterprise by them for more sustainability. If these inputs are not supported strongly then women are least likely to succeed in taking up any income generating activity on a sustainable basis even after having a desire and need for such activity. Based on Focused Group Discussion (FGD) role of NGOs in women empowerment has been highlighted here.

For centuries, women of the nation have stayed in the cave of societal taboos, have maintained their distinctive culture of living, have sustained on their family lives, and now they are struggling to overcome poor socio-economic condition. The women of this nation have stayed outside the realm of the self-motivation and self-reliance. Male dominated society for various needs, ranging from economic to social system has utilized women as the prime unit of child production. These concepts have been gradually integrated and incorporated in the social system of human beings. Domestic activities are often considered as the prime job of women. With innovative ideas and novel approaches, SHGscould be utilized as a change maker and could be a tool to provide better opportunities to the downtrodden. In this context SHGs have evolved some simple but innovative methodologies which could be a lesson to all.Failure stories could be helpful to revitalize the situation. By upholding the banner of Women

empowerment Vis-à-vis the success stories, the project reports of several NGOs, speaks of social, economic and political empowerment of womenthrough SHGs. Undoubtedly the civil society movement got huge success, followed by various entrepreneurial success and intends to highlight the success stories. Since the movement started, a bundle of failure stories are still sinking in the darkness.

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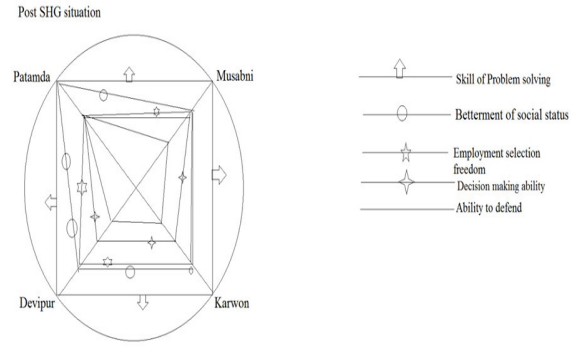

Figure 1 Cobweb Diagram of Social Empowerment

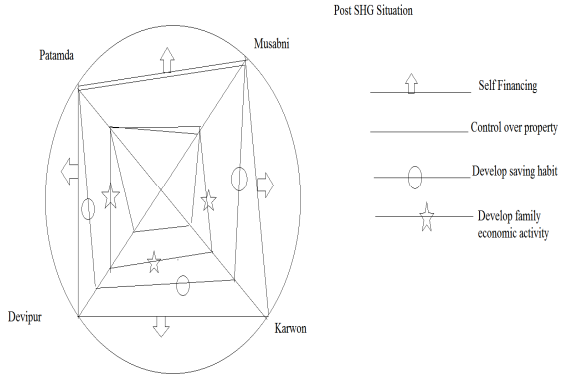

Figure 2 Cobweb Diagram: Economic Empowerment

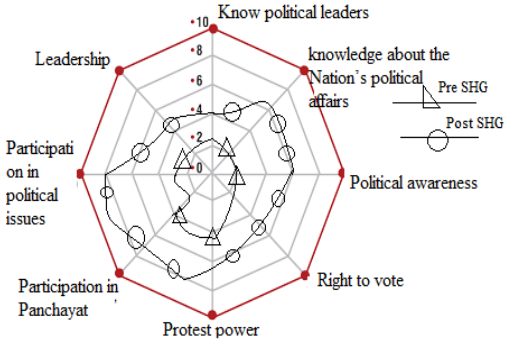

Figure 3 Spider Diagram: Political Empowerment

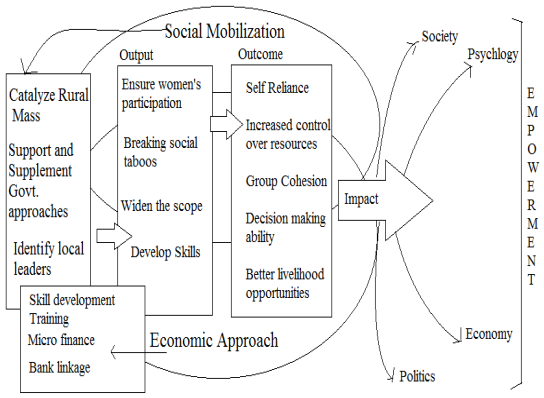

Figure 4 Role of NGOs in women empowerment

Table 1: Empowerment: Social point of view (Source: *Dr.Shivambhari Mishra viz. 'Empowering Men & Women Through Self Help Group'*

District	Blocks	GP	Respondents
East Singhbhum	Patamda	Bangurda	90
		Goberghuri	
	Musabni	Benashole	
		Bhobui	
Deoghar	Devipur	Dhobana	90
		Jhundi	
	Karwon	Badhanadih	
		Badia	
Total Respondents			**180**

Variables	Description
1. Skill of Problem solving	The capacity to resolve the problem of the family. Problems are related to social, economic & any other factors.
2. Betterment of social status	The members get social recognition, social understanding and higher social set up and higher place in the community. Anyone of these factors is considered improvement of social status.
3. Employment selection freedom	The women are free to select any employment channel according to their discretion.
4. Decision making ability	Decision making is mental process based on conscious reasoning. In this study, it refers to the participation of women of the family in making decision in all the important matters of home & economic activities.
5. Ability to defend	It is the ability or right to defend herself. The capacity is developed through SHG.

Table 2: Income of the SHG members before and after joining the SHGs

Sl.No.	Income (Rs/Month)	Before SHG		After SHG	
		No. of Respondents	Percentages	No. of Respondents	Percentages
1	Less than 1000	15	8.33	0	0
2	1000-2000	65	36.11	2	1.12
3	2000-3000	55	30.56	65	36.12
4	3000-4000	45	25.00	45	25.00
5	4000-5000	0	0	55	30.57
6	5000-6000	0	0	10	5.58
7	Above 6000	0	0	3	1.71

Table 3: Wilcoxon Signed Rank Test (Test statistics (b))

	Annual Income Before - Annual Income After
Z	-8.867[a]
Asymp. Sig. (2-tailed)	.000

Ranks

	N	Mean Rank	Sum Rank
Negative Ranks	100[a]		
Annual Income Before- Positive Ranks	0[b]	57.50	5750.00
Annual Income After Ties	0[c]	.00	.00
Total	100		

a. Annual Income Before < Annual Income After
b. Annual Income Before > Annual Income After
c. Annual Income Before = Annual Income After

I. **Cohesion Constraints of SHGs**:

Sl.No.	Constraints	Mean Score	Rank
1	Non-cooperation from family members	60.8	III
2	Poor leadership quality	64.3	II
3	Lack of trust on Group Leader	64.8	I
4	Women were very busy in their family works	53.2	IV
5	Non-cooperation from group members	45.2	v

II. **Group performance related constraints of SHGs**:

Sl.No.	Constraints	Mean Score	Rank
1	Lack of education	58.5	IV
2	Lack of fund	70.6	I
3	No exposure in record keeping	24.6	VI
4	Unskilled members/ Lack of training	59.9	III
5	Inability to loan repayment	43.5	v
6	Problem of marketing channel for the produce	67.4	II

III. Financial Constraints of SHGs:

Sl.No.	Constraints	Mean Score	Rank
1	Poor linkage with Bank	54.4	III
2	Inordinate delay in loan from bank	45.3	IV
3	Travel expenses for disbursement of loan	42.5	V
4	Irregular savings	62.6	II
5	Delay in loan repayment	68.3	I

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RESEARCH ARTICLE

Space Utilization Dimensions of Family Farms: A Case of East Singhbhum, Jharkhand

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ABSTRACT

Family based Farming System as a notion is fundamentally space related, time associated and relation oriented. But then, space related dimensions are intrinsic feature of Farming System Research. Actually, it deals with the consideration and analysis of spatial dimensions of farm and farm families. In its usual format, such an investigation gives elucidation how researcher synthesizes the characteristics of a farm in the light of peoples' veracities.Apart from such observations like; resource flow in a farm, the study intended to ventilate the diversity details of the farms. It can also be asserted that 'Space utilization pattern' of a farm deals with this aspect. In this way, the space utilization dynamics of the studied Family Farms can be synthesized.This study highlights the family farms of tribal farmers in East Singhbhum district of Jharkhand. Characterization of the farm resources and sustainability assessment of those farms are urgently needed, particularly in the context of natural resource management and socio-economic realities. Present study is descriptive in nature. The findings of this study have been discussed after analysis of the collected data through questionnaire and interview of the members of family farms and were subsequently summarized. PRA (Participatory Rural Appraisal) and FGD (Focused Group Discussion)are used here as a predominant methods of data collection. The findings had been summarized after throwing light on all the major aspects of the study. The conclusion and the suggestions were made to make the rural development possible through family farming.

Keywords: Family Farm, Space Utilization Pattern, PRA, FGD

INTRODUCTION

Everybody now consents to the way that expanding populace and land discontinuity will influence human oversaw agricultural frameworks also. Agricultural frameworks, specifically, is helpless against such changes. Since living has turned out to be more astonishing than some time recently, and also influences human need, particularly nourishment propensities, has likewise been moving quickly and among the general population agreement is progressing that by itself cultivating can't meet these developing requests of the general population by harvest development as it were. It needs enhancement with different endeavors in the basic agricultural frameworks to adapt up to this change.

Family farms allude to the homestead where in at least two differing financial actions are coordinated with farm/ agricultural assets for accomplishing their judicial use, acknowledge most extreme benefit and guarantee returns. Along these lines, the essential goal of the Farming System is to enhance quickly the financial states of individual homestead families by expanding change, heightening and expansion of various undertakings and generation wise sustainable methods; keeping in view the most recent advancements, requirements forced by assets, social taboos and the earth. Indian agriculture is not merely an occupation, but it is the way of life which for centuries has been shaped the life and out looks of the nation. It symbolizes peoples' struggle against economic deprivation. For centuries, tribes of this region have stayed in geographical isolation, have maintained their distinctive culture of farming, have sustained on subsistence family farms, and struggled to overcome poor socio-economic condition.Family Farming may be defined as the ''forms of organization of agricultural production and includes holdings that are characterized by organic links between the family and the production unit and by the mobilization of family labour, excluding permanent employees. These links are reflected in the inclusion of the productive capital in the family assets and in the combination of domestic and market and non-market operating logics in processes to assign family labour and for its remuneration, as well as in choices for the distribution of products between final consumption, intermediate consumption, investments and accumulation'' (Bélières et. al, 2015).It is understood that with rising population, declining land-man ratio and dwindling of land and labour productivity, agriculture alone would not able to provide adequate income and employment to households in India. Further, there is hardly any scope for horizontal expansion of land and only vertical expansion is possible by integrating various farm enterprises. Under such circumstances, to ensure a regular flow of income for decent living and to achieve food and nutritional security, farmers have to undertake some land based enterprises which will complement existing farming activity to get more income leading to social and economic upliftment (Behera et al., 2001).A predictable reaction of farming extension and strengthening has been the fracture and disconnection of normal natural surroundings inside an inexorably inadmissible lattice for some species (Donald et al., 2001). Natural surroundings discontinuity and its belongings prompt a scope of environmental and biological system changes. Among these, biodiversity characteristics, for example, species arrangement, group structure, populace elements, conduct, reproducing achievement, and individual wellness are adversely influenced (Silva and Pontes, 2008).Altieri (1987) reported that consequences of biodiversity are nowhere more evident than in the realm of agricultural pest management. Further, it was reported that the instability of agro ecosystems increases with the worsening of most insect pest problems, which is increasingly linked to the expansion of crop monoculture at the expense of the natural vegetation and thereby decreasing local habitat biodiversity. Desai et al. (1995) opined that occupational structure reflects economic sustainability of any region in terms of type of work, level and skill of workers, number of days that workers are employed in work per year, nature of work, full time versus marginal work etc. It is also important to know the level of occupational sustainability of a region, both at a macro and at a micro level, over a period of years in order to ascertain its economic development. Sivananthan and Subramaniam (1995) reported that, in India where small and marginal farmers are predominant were operating only at low level of output and productivity. This was due to rapid increase in input prices and relatively fluctuating prices of output.

Objectives of the study : The study intends to ventilate-

1. To characterize the family farms
2. To trace out space utilization pattern

METHODOLOGY

This study is an amalgamation of descriptive research, correlational study and exploratory research.This study is a blending of structured and unstructured approach.

Sample size: 270 samples were drawn by using Multistage Purposive Sampling.

Sampling Design: From the district, 3 blocks having >60% tribal population had been selected. Thereafter, 3 villages were selected from each block. After that, 30 farmers were selected from each village.

SELECTION OF THE STUDY AREA

1. **Selection of the district:** Jharkhand is comprised of 27 districts. Out of this one district namely East Singhbhum was conveniently selected for the present study.
2. **Selection of the block:** There are 11 blocks in Deoghar district. Out of these 11 blocks, three blocks namely Ghatshila, Patamda and Baharagora block were purposively selected for the study.
3. **Selection of village:**Darisai, Bodhpur and Bhamradih villages of Ghatshila block, Dongagarh, Dhatkidih and Loraidoongri villages of Patamda block, Jarabani, Pochakhuli and Satpati villages of Bharagora block were selected.

RESULTS AND DISCUSSION

Characterization of Family Farms

After a focused group discussion (FGD) conducted with the farm dwellers, five types of Family based Farming Systems were identified (Table No. 2). The classification was largely based on different components of the system. The classification is an output of thorough, on-the-spot personal interview vis-à-vis focused group discussion (FGD). Data collected through interview schedule was discussed with the key informants of the three blocks. At this stage, the credential of this classification was further consulted with the experts. The details of the types of Family Farms followed by the respondents were also investigated. Four types of Family Farms were identified in the study area.

It is noted from the table 2; that the Type I, which is comprised of crop, cattle, poultry, goatery vegetable and fruit crops, were 22.22% of all the farms. Type II farms (17.03%) comprised of crop, cattle, poultry, fishery, vegetable and fruit crops. Type III farms (18.52%) comprised of crop, cattle, and goattery which did not have conspicuous presence of horticulture components. But they have small homestead vegetable gardens. Type IV (22.22%) was devoid of poultry and goatery component while Type V (20%) had fishery component.

Diversity details (biodiversity and crop diversity) of different types of Family Farms:

Apart from such observations like; resource flow in a farm, the study intended to ventilate the diversity details of the farms. It can also be asserted that 'Space utilization pattern' of a farm deals with this aspect. In this way, the space utilization dynamics of the studied Family Farms can be synthesized.

Table 3 describes the diversity details of different types of Family Farms. Highest number of trees was recorded in Farm Type IV. However, number of trees/ acre was highest in Farm Type IV, Followed by Farm Type I. These two farms have vegetables and fruits as an integral part and hence the higher number of trees is expected. Farm type IV had forestry component with it.

Highest number of tree species was recorded in Farm Type IV followed by Farm Type I. Biodiversity measured by Simpson Index and Shanon Index was found highest in Farm Type IV followed by Farm Type II.

Energy consumption and energy input-output relationship in different farms:

Table 4.1.2.6 shows the details of input use and output gain from the family farms. The quantity of input and output multiplied by their energy equivalents generated the energy input-output scenario of the family farms. The major sources of energy input of these farms were nitrogenous fertilizers, followed by irrigation, power tiller and human labour. Energy input required per unit area was lowest for farm type V, followed by farm type IV and I. This was perhaps due to the presents of farm components that required lesser energy input like- nitrogenous fertilizer. Energy efficiency was also found to be highest for farm type V, followed by farm type I and II.

Mandal, Saha, Ghosh, Hati and Bandyopadhyay (2002) opined that energy input–output connections in trimming frameworks fluctuate with products being developed in arrangement, by sort of soils, nature of culturing operations for seedbed planning, nature and measure of natural compost, substance manure, plant insurance measures, reaping and sifting operations and, at last, yield levels.

Farming is both a maker and purchaser of vitality. It utilizes expansive amounts of locally accessible non-business vitality, for example, seed, excrement and enliven vitality, and in addition business energies, straightforwardly and in a roundabout way, as Diesel, power, manure, plant insurance, compound, water system water, hardware and so forth. Proficient utilization of these energies accomplishes expanded creation and efficiency and adds to the productivity and intensity of horticulture maintainability in provincial living (Singh, Mishra and Nahar, 2002).

Carbon stored (mt) in the woodlot in different family farms

Table 5 describes the carbon storing as a part of ecosystem is considered as an important strategy for reducing greenhouse gas emission to atmosphere. Tree biomass per unit area was found highest in farm type II, followed by farm type I and IV. The carbon storage of per unit area also followed the same pattern in farm type I, II and III. Horticulture, fruit trees and agroforestry are important components and hence, higher biomass and carbon storage also found in those farms.

CONCLUSION

The farm dwellers, particularly the small farmers of our nation, are defied with numerous financial, input oriented, institutional, regulatory and technical limitations obstructing the growth of farm income and in this way compelling them to live in distressful condition. The declining pattern in size of land holding represents a genuine test to the maintainability and benefit of farming. Along these lines, it is normal that no single endeavor can produce sufficient pay and work during the time to keep up a base way of life of ranchers, especially the small and marginal farmers of state.Data collected through household survey, FGD, PRA from three selected blocks of East Singhbhum namely, Ghatshila, Patamda and Bahragora revealed the followings: After focused group discussion (FGD) conducted with the farm dwellers, five types of Family based Farming Systems were identified. (Family farm type I= Crop + Cattle + Poultry + Goatery+ Vegetable + Fruits, Family farm type II= Crop + Cattle + Poultry + Fishery + Vegetable + Fruits, Family farm type III=Crop + Cattle + Goatery + Vegetable, Family farm type IV=Crop + Cattle + Vegetable + Fruits/ Forestry, Family farm type V=Crop + Cattle + Poultry + Fishery + Vegetable). Highest number of trees was recorded in Farm Type IV. However, number of trees/ acre was highest in Farm Type IV, Followed by Farm Type I. These two farms have vegetables and fruits as an integral part and hence the higher number of trees is expected. Farm type IV had forestry component with it. Highest number of tree species was recorded in Farm Type IV followed by Farm Type I. Biodiversity measured by Simpson Index and Shanon Index was found highest in Farm Type IV followed by Farm Type II. A blend of enterprises like fishery, poultry, forestry alongside yield development and so forth is important to beat the issues confronted by the asset poor agriculturists, i.e. farming system approach in dealing with the accessible assets is accepted to have the probability to haul out the farmers from the endless loop of neediness. The family based farming system reasonably is an arrangement of components or enterprises, which are interrelated and connect among themselves in getting assets and conveying yields to the common condition. At the focal point of collaboration are simply the farmers in practicing control and access on decision of the sort and aftereffects of such different institutions.

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Table 1: Selection of the study area

State	District	Blocks	Villages
Jharkhand	East Singhbhum	Ghatshila	Darisai, Bodhpur, Bhamradih
		Patamda	Dongagarh, Dhatkidih, Loraidoongri
		Bahragora	Jarabani, Pochakhuli, Satpati

Table 2: Distribution of different types of Family based Farms

Farm Type (Enterprises)	Nomenclature	Frequency
Crop + Cattle + Poultry + Goatery+ Vegetable + Fruits	Farm Type I	60 (22.22)*
Crop + Cattle + Poultry + Fishery + Vegetable + Fruits	Farm Type II	46 (17.03)
Crop + Cattle + Goatery + Vegetable	Farm Type III	50 (18.52)
Crop + Cattle + Vegetable + Fruits/ Forestry	Farm Type IV	60 (22.22)
Crop + Cattle + Poultry + Fishery + Vegetable	Farm Type V	54 (20)

Note: *Figures in the parentheses indicate the percentage to total*

Table 3:Diversity details (biodiversity and crop diversity) of different types of Family Farms

	Farm Type-I	**Farm Type-II**	**Farm Type-III**	**Farm Type-IV**	**Farm Type-V**	**Overall**
No. of trees	M-87.67 SD-43.98	M-178.67 SD-124.18	M-127.43 SD-81.81	M-190.14 SD-126.37	M-119.00 SD-84.19	M-146.37 SD-103.06
Rank	**V**	**II**	**III**	**I**	**IV**	
No. of trees per Acre	M-41.47 SD-27.69	M-19.61 SD-17.85	M-31.55 SD-28.42	M-15.71 SD-13.21	M-50.26 SD-36.88	M-33.24 SD-28.14
Rank	**II**	**IV**	**III**	**V**	**I**	

No. of trees per species	M-16.71 SD-2.87	M-15.17 SD-4.40	M-12.14 SD-4.56	M-17.14 SD-5.79	M-14.00 SD-1.00	M-15.17 SD-4.500
Rank	V	III	V	I	IV	
Biodiversity (tree) (Simpson Index)	M-0.79 SD-0.05	M-0.74 SD-0.03	M-0.77 SD-0.14	M-0.80 SD-0.11	M-0.83 SD-0.10	M-0.78 SD-0.09
Rank	**III**	**V**	**IV**	**II**	**I**	
Biodiversity (tree) (Shannon-Weiner Index)	M-1.97 SD-0.15	M-2.00 SD-0.27	M-1.82 SD-0.51	M-2.20 SD-0.38	M-1.75 SD-0.16	M-1.95 SD-0.35
Rank	**III**	**II**	**IV**	**I**	**V**	
Crop Diversity	M-0.72 SD-0.18	M-0.75 SD-0.17	M-0.63 SD-0.23	M-0.74 SD-0.23	M-0.69 SD-0.23	M-0.70 SD-0.19
Rank	**II**	**V**	**I**	**IV**	**II**	

Table 4: Energy consumption and energy input-output relationship in different farms

Input head	**Farm Type I**		**Farm Type II**		**Farm Type III**		**Farm Type IV**		**Farm Type V**		**Overall**	
	Quantity	Total Energy Equivalent	Quantity	Total Energy Equivalent	Quantity	Total Energy Equivalent	Quantity	Total Energy Equivalent	Quantity	Total Energy Equivalent	Quantity	Total Energy Equivalent
Human Labour (Man Hour	306.2	600.32	525.28	390.8	766.08	522.6	1024.40	442.2	866.88	317.73	728.70	728.70
Bullock Labour (Hr)	8.00	80.80	6.33	63.97	9.14	92.34	12.00	121.20	9.71	98.11	8.73	88.21
Seed(kg)	32.31	475.06	23.25	341.80	34.30	504.15	47.76	702.12	43.27	636.03	35.07	515.46
N Fertilizer(kg)	44.44	2693.2	32.04	1941.6	50.85	3081.8	60.91	3691.3	69.90	4235.8	51.04	3093.3
P Fertilizer(kg)	17.46	193.77	11.45	127.09	17.37	192.8	21.63	240.1	30.18	335.1	19.62	217.8
K Fertilizer(kg)	17.53	117.44	14.85	99.50	22.54	151.04	14.40	96.48	24.49	164.10	19.48	130.48
Pesticide(g;ml)	1.26	15.07	0.29	3.46	0.61	7.29	2.46	29.56	2.37	28.49	1.29	15.51
Irrigation(hr); in Diesel Equivalent	25.14	1576.5	19.67	1233.1	44.14	2767.8	51.67	3239.5	37.43	2346.8	34.00	2131.8
Total Energy Input(MJ)		6383.6		4790.4		8247.3		10085.0		9571.1		7613.7
Energy/Unit Area		1261.5		1320.3		1768.6		1243.8		1130.9		1359.3
Rank		**3**		**4**		**5**		**2**		**1**		
Total Energy Output(MJ)		101831.31		59851.87		98484.84		131758.17		138224.76		104139.07
Energy Efficiency		16.04		13.23		13.15		11.18		16.30		14.38
Rank For Energy Efficiency		**2**		**3**		**4**		**5**		**1**		
Water used per unit Biomass(L/Kg)		0.08		0.07		0.07		0.04		0.09		0.07
Rank		**2**		**3**		**3**		**4**		**1**		

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RESEARCH ARTICLE

Temporal Dimensions of Family Farms: Looming Lights on East Singhbhum, Jharkhand

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ABSTRACT

For centuries, tribes of the 'Chotanagpur Plateau' region have stayed in geographical isolation, have maintained their distinctive culture of farming, have sustained on family farms, and struggled to overcome poor socio-economic condition. The tribal groups of this region have stayed outside the realm of the developmental outputs because they reside in forests and hilly tracts. On the other hand, the plateau of Jharkhand is popular for its mineral resources. Industries often consider these people as the passive resources. They have been used as cheap labour forces. As a result their condition was in doldrums. On the other hand, tribal communities are maintaining their indigenous farming. Tribal farming is not merely an occupation but it is the way of life, which for centuries has been shaped their lives and livelihood. They are dependent on small farms, which were maintained by the family members. The study is the modest endeavour to highlight the temporal dimensions of the family farms. The data was collected through questionnaire and interview with the participants and the collected data was analysed to discuss and summarised it's outcomes. PRA (Participatory Rural Appraisal) and FGD (Focused Group Discussion) are used here as a predominant methods of data collection. The findings had been summarized after throwing light on all the major aspects of the study. The conclusion and the suggestions were made to make the rural development possible through family farming.

Keywords: Family Farming, Temporal Dimension, PRA, Jharkhand, Tribal Agriculture

INTRODUCTION

Temporal dimensions of family farms deal with the time related facets of family farms in farm realities. It consents the farmers to express their perceptions about various cumulative incidents and impacts on farms over a period of time. The temporal dimensions of farms inside the natural examination remained generally inside the breaking points of the progressing time frame. The assessment is more about the recognition of negligence in natural generation than discovering deficiencies in the expert abilities of the farmers.

Critical advance likewise was made in growing more proper strategies to break down the aftereffects of farming system research and make suggestions in view of them. Two methodologies that merit extraordinary say are: flexibility (in the past, altered dependability) investigation which has turned out to be an especially profitable measurable device for examining consequences of on-farm trials, especially those that include farm usage or both agriculturist administration and execution (Hildebrand and Russell, 1996).

At the mid to late 1980s, some huge methodological and institutional advancement were presented in the execution of the farming system approach with an entire highlighted aspects.

One has included advancement and usage of philosophies to work with agriculturists to evaluate bio-resource (supplement) patterns and streams at the ranch family unit level. The thought is to decide biomass slants after some time and to help recognize, with the agriculturist, powerless parts of the cultivating framework for which changed techniques are expected to advance biological maintainability. Huge numbers of these methods have their root in RRA/PRA (Lightfoot, Bottrall et al., 1991).

For centuries, tribes of the 'Chotanagpur Plateau' region have stayed in geographical isolation, have maintained their distinctive culture of farming, have sustained on family farms, and struggled to overcome poor socio-economic condition. The tribal groups of this region have stayed outside the realm of the developmental outputs because they reside in forests and hilly tracts. On the other hand, the plateau of Jharkhand is popular for its mineral resources. Industries often consider these people as the passive resources. They have been used as cheap labour forces. As a result their condition was in doldrums. On the other hand, tribal communities are maintaining their indigenous farming. Tribal farming is not merely an occupation but it is the way of life, which for centuries has been shaped their lives and livelihood. They are dependent on small farms, which were maintained by the family members.

METHODOLOGY

This study is an amalgamation of descriptive research, correlational study and exploratory research.This study is a blending of structured and unstructured approach.

Sample size: 270 samples were drawn by using Multistage Purposive Sampling.

Sampling Design: From the district, 3 blocks having >60% tribal population had been selected. Thereafter, 3 villages were selected from each block. After that, 30 farmers were selected from each village.

SELECTION OF THE STUDY AREA

1. **Selection of the district:** Jharkhand is comprised of 27 districts. Out of this one district namely East Singhbhum was conveniently selected for the present study.
2. **Selection of the block:** There are 11 blocks in Deoghar district. Out of these 11 blocks, three blocks namely Ghatshila, Patamda and Baharagora block were purposively selected for the study.
3. **Selection of village:** Darisai, Bodhpur and Bhamradih villages of Ghatshila block, Dongagarh, Dhatkidih and Loraidoongri villages of Patamda block, Jarabani, Pochakhuli and Satpati villages of Bharagora block were selected.

RESULTS AND DISCUSSION

Historical Transect of the family farms

Historical Transect is a PRA method which was used to reconnoitre the temporal aspects of the family farms. It revealed the changes in farm resources over a period of time. During PRA, discussion with the key- informants explored the causes behind the changes in farm over time. Figure 1 was an output of the cumulating result (of three blocks) of discussion. Thereafter, overall changes were represented through spider diagram.

Figure 1 covers various aspects of family based farms like- crop diversity, livestock, water resources and yield. The time line transect of the figure segregates the history in six fold of times- before 1950, 1950, 1970, 1990, 2000 and after 2000. A glance on the figure would create a clear idea about the major changes in family farms over time. It is clear from the figure – During 1950, crop diversity was reduced in farms. Discussion with the key-informants also revealed that because of scarcity of rain fall yield was also reduced during this period of time. This area faced severe drought condition during this period of time. After that, aspects like-crop diversity, livestock and yield were increased but water level was decreasing day by day. During 1990s, tube/ bore well and other water structures were installed in the study area.

The crop diversities were come down during 1950s. It happened because of mono-cropping of paddy. From 1970s, crop diversity was increased. To some extent some vegetables were grown along with paddy. The positive side, revealed from the discussion was that villagers were quite optimistic about the future of their family farms. The study revealed that condition of ground water was quite alarming. Gambling of monsoon and decline in ground water level might create hindrance in their farm sustainability.

The transcription of FGD was thoroughly analysed. Figure 2 was an output of the analysis. From this figure, historical events could be clearly understood. The aspects which had major impact on family based farms were discussed and expressed in the light of timeline. The outcomes of the discussion were compressed in Figure 2.

Seasonal analysis: Food Availability in Family Farms

Seasonal diagram is an output of seasonal analysis, done by the dwellers of the farm families. The special focus of this analysis was to ventilate the relationship between food availability and season. From the diagram it was found that during three month's lean (March-June) period, farm dwellers used to face food scarcity.

Food security has remained one of the most important concerns of the study area because of its scattered rainfall. Figure 3 gives an overall idea about the extent of food security across the season. Table 1 provides an idea of food consumption by the household under different types of family farms. Rice is the most important source of carbohydrates. For most of the households in all types farming system, food was available throughout the year. Farm type I, II and V were most assured of food items on their own farms than the other farm types.

CONCLUSION

The farm dwellers, particularly the small farmers of our nation, are defied with numerous financial, input oriented, institutional, regulatory and technical limitations obstructing the growth of farm income and in this way compelling them to live in distressful condition. The declining pattern in size of land holding represents a genuine test to the maintainability and benefit of farming. Along these lines, it is normal that no single endeavour can produce sufficient pay and work during the time to keep up a base way of life of ranchers, especially the small and marginal farmers of state. Everyone now agrees to the fact that increasing population and land fragmentation is going to affect human managed systems as well. Farming systems, in particular, is vulnerable to such changes. Since living has become more complex than before, human need, specifically food habits, has also been shifting rapidly and among the people consensus is on the move that alone farming cannot meet these growing demands of the people by crop cultivation only. It needs diversification with other enterprises in the farming systems to cope up with this change. Chotanagpur Plateau region, study area, is feared to be worst affected by such changes as along with anthropogenic

changes societal variations are very prominent in the area and hence need alternative livelihood strategies to reduce the odd impacts on the farming systems of this region.

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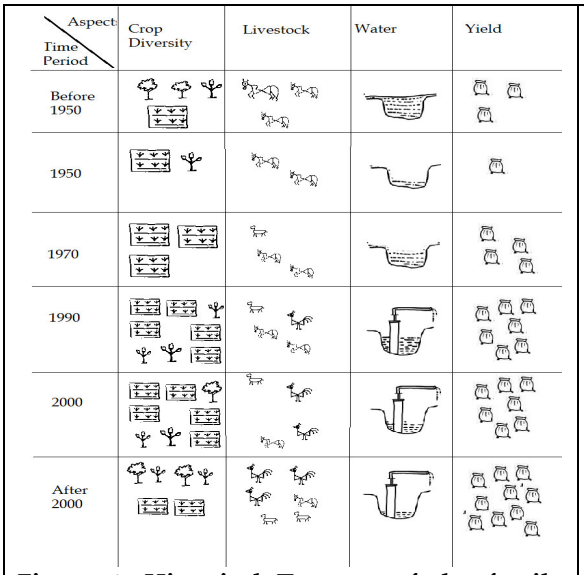

Figure 1: Historical Transect of the family farms

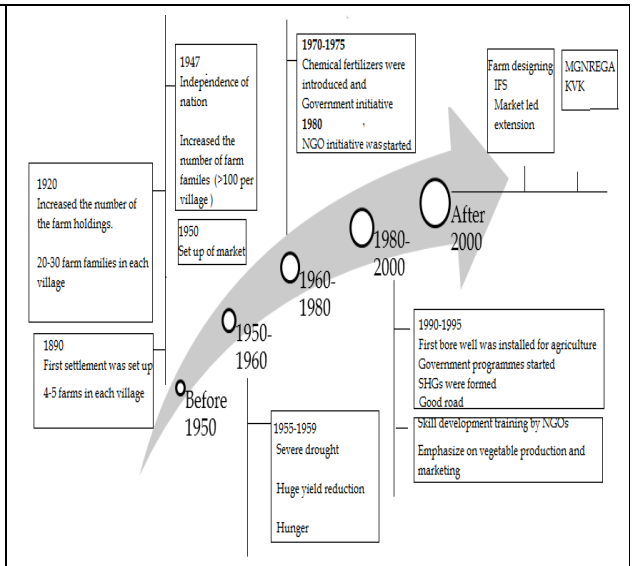

Figure 2: Historical timeline of the family farms

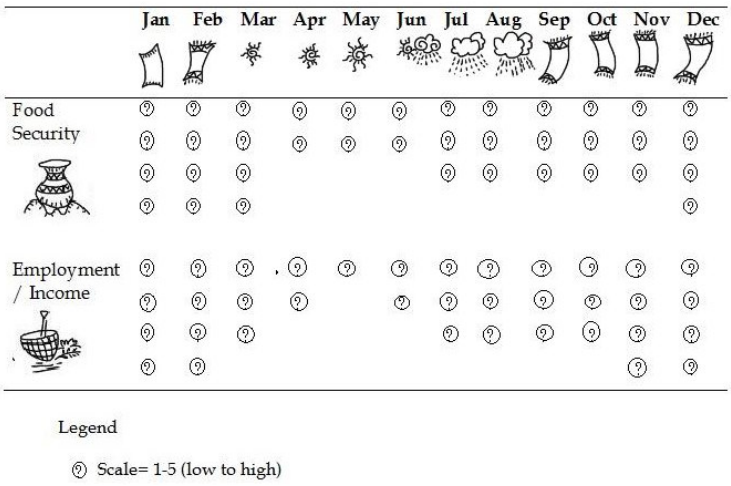

Figure 3: Seasonal analysis of food availability

Table 1: Selection of the study area

State	District	Blocks	Villages
Jharkhand	East Singhbhum	Ghatshila	Darisai, Bodhpur, Bhamradih
		Patamda	Dongagarh, Dhatkidih, Loraidoongri
		Bahragora	Jarabani, Pochakhuli, Satpati

Table 2: Availability of food from the family farms for household consumption need

	Farm Type-I	Farm Type-II	Farm Type-III	Farm Type-IV	Farm Type-V	Overall
For 9 months	5 (8.33)	11 (23.92)	20 (40.00)	25(41.66)	4 (7.41)	65(24.08)
For 12 months	55(91.67)	35(76.08)	30(60.00)	35(58.34)	50(92.59)	205(75.92)
Rank	**II**	**III**	**IV**	**V**	**I**	

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RESEARCH ARTICLE

Urbanization: Changes in the Socio Economic Condition of the Tribes (Bhumij)

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ABSTRACT

The paper entitled "Urbanization: Changes in the Socio-Economic condition of the tribes (Bhumij)" is a modest endeavor to highlight the Impact of urbanization on the tribes (Bhumij) of Lowakui, Purulia. Scheduled Tribes (STs) are indigenous, have their own distinctive culture, geographically isolated and are low in socio-economic conditions. For centuries, the tribal groups have remained outside the realm of the general development process due to their habitation in forests and hilly tracts.Ever-since India embarked on the path of developmental planning there started a series of infrastructure projects, be it Basic and Heavy industries. Industrialization and urbanization stimulate migration. Apart from migrating 'Bhumijs' from their ancestral 'Tanda' (Colony) and 'severing their cultural ties and bonds established over generations', migration also devastates the social life of them. 'Quantitative as well as Qualitative approach has been adopted for the study. 'Participatory Rural Appraisal' and 'Case Study' are the integral part of the research work. The study also thoroughly analyses the constraints face by the migrated Bhumijs. Case study method plays a vital role to realize their situation. Some case studies reflect the physical and sexual exploitation of the migrated tribal women. The study provides a snapshot of the critical issues affecting the traditional tribal culture and society. Finally, the study has tried to provide concrete and useful suggestions for the tribal development.

Keywords: Urbanization,Industrialization, Socio economic lives, Physical and sexual exploitation, Migration, Quanti-Quali approach, 'Participatory Rural Appraisal' and 'Case Study'

INTRODUCTION

Jojo (2003) opined that after independence, capital intensive establishments were considered as *modern temples* of India. Baxi (2008) has been shown that no development without displacement became the *mantra* of developers everywhere. The tribal communities generally dependent on Forest- Hunting, Hill Cultivation, Plain Agriculture, Simple artisan and Folk Art etc. Due to urbanization, many of the tribal are migrating to different industrial belts and towns. Nature and natural resources are now treated as the 'Passive Resources'. It is because of industrialization, urbanization and its natural consequences. Expansion of urban areas and deforestation is going on parallely. These types of incidence have changed the definition of the tribal life. Tribal society is largely egalitarian and tribal women have been equal partners withtribal families and have the contribution to household economy. Quite often their women do more physical labour in their agricultural fields and forest than that of the tribal men. Society for Regional Research and Analysis (2010) opines that it has been observed that large number of educated, uneducated and illiterate tribal women from Jharkhand, Chhattisgarh, Orissa and West Bengal migrate to different parts of country and metropolitan city like Delhi, Mumbai, Kolkata are their major destinations for searching some gainful employment/casual labour in the unorganized sector and as household maids for their livelihood. They are often exploited physically and sexually. These types of incidence have changed the definition of the tribal life. Oomen (2004) opined that thus, the rural was to be displaced by the urban; agriculture by industry; low, simple, or traditional technology by high, complex, or modern technology. But the obsession with a particular pattern of development and the displacement it entails whereby the green fields (belonging to people) are being turned into Greenfield (or such corporate hubs with ironically misleading names) – is playing havoc with the lives of large number of people and, hence the need to turn the spotlight on it.

The plateau of Chotanagpur is not only popular because of abundance of mineral resources but also popular as it is the dwelling place of various tribes. Mainly 'Protoaustraloid' tribes are sprung from the earth of Chotanagpur plateau. They have their own lifestyle and culture. Their lives and livelihoods were mostly dependent upon nature and natural resources. There was a reciprocal relationship between nature and the tribes.

Brief note about the Bhumijs

Bhumijdepicts one who is born from the soil. They form one of the Hinduised Adivasi groups inChotanagpurplateau. They are Austric-speaking people who have adopted Bengali as their second language due to their contact with the Bengali-speaking people of Purulia district of West Bengal. Generally, Bhumij family is patrilineal type. Monogamy marriage is their tradition. But Bigamy/ Plygamyis not prohibited. Levirate and Sororal marriages are not also restricted. However premarital relations within the lineage group are prohibited. Marriage may take place between boys and girls of two different lineage groups but it is avoided.

Forest product and agriculture produce are main source of livelihood of them. They have a strong believe in animism and they also practice ancestral worship. They believe in naturalism and worship objects like animal, birds, sun, river, mountain, tree, plants and bushes. The Bhumij landholders rose to the status of feudal chiefs and then to the status of kings claimed themselves as Kshatriyas of Solar or Lunar dynasties.

Objectives of the study

Keeping the aforesaid objectives in view and looking at impact of urbanization on the socio economic lives of the Bhumijfrom Lowakui, a study was conducted to find out:

1. To understand the impact of urbanization on the socio-economic lives of the Bhumijs
2. To find out the sufferings of the migratedBhumij women.
3. To perceive the perception of the Bhumijs about the impact of urbanization.

The empirical study was conducted with a broader objective *to bring desired positive changes among the tribes.*

Research design

The present study is a comparative and descriptive one. The study is also based on Ex- post facto research design. Based on the research problems, specific objectives were decided. Basically based on review of literature, the problem and related issues were understood. After that, the process of data collection was started.

Locale of the study area: The present study was conducted at the picturesque hamlet of Lowakui (Block: Baghmundi, Dist: Purulia, State: West Bengal). It is about 40 kms from Purulia town via Balarampur. It is 10 kms away from Baghmundi. The village is nearer to famous 'Ayodhya' hill. It is 2133 ft above sea level. It is located close to Charida village also. The village situates under the jurisdiction of 'Matha Forest Range.

S**ample size :(n)** of the study was **75 from 25 families.** In order to select the sample**, purposive sampling was done.**

Study period: The study period was from 11th September, 2012 to 11th August,2013.

The methods of data collection were both quantitative and qualitative in nature and were aimed to seek answers to certain research questions which would be deducted from various studies, researches and also during the field study. Given below is a list of the major techniques of data collection utilized by the

Researcher-author for the present study

1. Interview
2. Observation (Participant Observation and Non-Participant Observation)
3. Case Study
4. Focused Group Discussion (FGD)
5. Participatory Rural Appraisal (PRA)

The findings of this study had been discussed after analysis of the collected data and were subsequently summarized. The conclusion and the suggestions were aiming to bring desired positive changes among the tribal community.

Key findings: Impact of urbanization on the socio economic lives of the Bhumijs

Findings: In the light of Objective 1: To understand the impact of urbanization on the socio-economic lives of the Bhumijs.

The economic life of the tribes is specific in nature. Their social life also varies from one to another. The independent variables which were taken for measuring the findings of the research were age, family size, family education index, family occupation, individual income. Rather than these Socioeconomic Status Scale of Kupuswamy, (1976) is used to measure the socio economic condition of the study area.

Figure 1 reveals that large land owners have a trend not to work at Mines of Asansole. They generally migrated to Asansole ,Bokaro and Tatanagar. Those who have large land holdings; they are generally involved in Agriculture. Landless respondents have a trend to work as Mine labours and labours.

As they have large land holdings, they are generally involved in Agriculture. Landless respondents have a trend to work as Mine labours and labours. This reveals that those have small land holdings; they are prone to work in the mines.

Decline in Joint Family: Bhumijsettlements are known as Tandas. Their society is largely egalitarian. The female candidates migrated with their husbands. They used to live at the urban slams of Assansol, Bokaro and Tatanagar for that particular season, nearer to the Industrial belt. The result of PRA was also showing the same trend of breaking down of joint family to nuclear families.

Acculturation and detribalization: Tribal cultures have evolved over millennia in their particular habitats and environment. Most of them have evolved in isolation as the interaction between tribals and non-tribals have been minimal. These customs and beliefs are different from the mainstream cultures.

Most of the migrated respondents are working in the industries as casual labours. They are devoid of any type of care and protection. They are influenced by the urban culture. Finally it affects the root of the tribal culture. Along with these, industrialization has changed their socio-economic condition. As a result of industrialization and migration, the tribal communities are adopting the modern culture and life style. Their source of income is changing. They become more vulnerable and dependent on industry. Trend analysis shows that Women become more vulnerable. They are treated as easily available commodities. Women are now trying to be a part of the 'Babu' culture. They are adopting Hindu rituals and customs. Those who are residing nearer to the industry, they often influenced by the urban/industrial culture. Electronic media (like; TV) also plays a vital role in 'Detribalization' process

Table 2 shows that there is a statistically significant relationship between then involvement in traditional programme and distance from the urban area. The Bhumij communities generally dependent on Forest- Hunting, rope making etc. However, due to industrialization/ urbanization, many of them are migrating to industrial belt of Assansol, Bokaro, Tatanagar. Some of them are living in the close proximity of the industries. They are working in the industries as casual labours. They are devoid of any type of care and protection. They are influenced by the urban culture. Finally it affects the root of the tribalculture. Along with these, urbanization has changed their socio-economiccondition. As a result of urbanization and industrialization, the tribal communities are adopting themodern culture and life style. Their source of income is changing. They become more vulnerable and dependent on industry. Women become more vulnerable. They are treated as easily available commodities. Hence, the Bhumijs, who migrated from Lowakui, avoid their cultural norms. It is because of acculturation and Sanskritization. But the Bhumijs of Lowakui lived in a isolated forest fringe area. Hence, the impact of industrialization and urbanization is less on their socio-cultural lives and it helps them to sustain 'Bhumij-hood'.

Improvement of economic condition

t-Test: Paired Two Sample for Means

From the output of the above table, it is observed that the p-value for two-tail test

(1.1714E-06) is less than the specified level of significance (0.05). So we **fail to accept**

Null Hypothesis (H0) and accept the Alternative Hypothesis (H1)

Hence, from the above decision, we can conclude that the difference between income (in Rs.) before and after getting migrated at Towns/ urban areas is statistically significant. Hence, we can interpret that after industrialization there has been a significant increase in the average income of a migrantBhumijs.

From the output of the table, it is observed that the p-value for two-tail test (0.072245914) is greater than the specified level of significance (0.05). So we accept Null Hypothesis (H0).

Hence, from the above decision, it can be concluded that the difference of income (in Rs.) before and after 10 years (people living at Lowakui) is not statistically significant. Hence, it can be interpreted that after urbanization there has not been a significant increase in the average income of Bhumijs of Lowakui.

When all of them used to live atLowakui, they had their primitive economy. They were though broadly branded as hunter-gatherers. The Bhumijs collect jungle products and exchange them with the neighbouring settled Hindu peasants for their day-to-day livelihood. Massive investment in urbanization and industrialization create wealth to the nation and employment opportunities to various people. It also happened at Assansol, Bokaro, Tatanagar and other industrial belts, nearer to Purulia. Those who migrated to the urban areas, their economy has been changed. They are often willing to take on jobs that others cannot or do not want to do (those that are dangerous; like mine

labours, brick industry labours, construction labours etc.). Although the work is insecure and nominal paid but it is very essential for them who are from marginal areas where wages are too low to make a living. Income is one driver, with people migrating in search of paid employment. Because of this paid employment, they are getting regular income. But the Bhumijs of the Lowakui is dependent upon their traditional economy. Along with this their traditional economy is also hampered because of implementation of new forest laws.

Findings: In the light of Objective 2: To find out the sufferings of the migrated Bhumijwomen

Exploitation of the women:

'A new feature of tribal migration from Lowakuiin recent yearshas been the large - scale migration of single women to cities in search of livelihood, which is a subtle change from the earlier migration patterns when only the men migrated to urban centres/ industries. Bhumijfamilies nowadays are driven by poverty to send unmarried daughters/ married wife to cities in search of work. Single women and tribal girls are however, prone to exploitation not only by employers but also by anti-social elements.' Tribal migrant women exploitation is mostly done by the middlemen who offer them good emoluments, good placement and work conditions and after they are taken to the work place they are cheated.

The specific case of PhoolmaniSing Mura could enlighten the issue. Present author talked with her. The summery of the conservation could be included.

Specific case

Name: PhulmoniSing Mura / Name of the husband: BudhiaSing Mura / Children: Four Sons / Age: 55 years

Phulmoni of Phuldungri is illiterate. Her parents did not send her to school. It is not a matter of regret to her. She says that today's girls of Lowakuiare also going to school. As a result their household activity is being reduced. Electricity facility is available now. Hence, girls watch TV throughout the day. They are influenced by the TV heroines.

Their social lives have been changed. This is because of urbanization. She believes that people has lost their 'Bhumij-hood'. There is no real Bhumij atPurulia city!!!

Phulmoni opined that electricity facility was not available in that time atLowakui. Hence TV was not also available. She added, 'they were the real Birhors'! The word 'they' denotes the earlier inhabitants ofLowakui. Those who live in city, consider themselves as the 'Hindu'. Phulmoni knows that caste cannot be changed. Caste membership cannot be achieved as it is the ascribed status. They are not the Hindu also. It is an imitation.

The girls were not sent to cities as because they were often being exploited. But now a day they are going to work in the cities. Their parents send them to work in brick-factories.

The daughter of Phulmoni also went to Tatanagar. She was a construction labour. The agent of the labours was a lascivious person. The women labours were often exploited because of his debauchery. Phulmoni's daughter was not an exception. Her husband knew everything. But he was an avaricious person.

Avarice leads to vice, and vice leads to death. At last she committed suicide. Local newspaper covered the news. Phulmani's eyes bathed in tears……

Economic exploitation: They often exploited by the labour agents. They are economically exploited. The payment is also irregular. They were economically deprived against their toils. The recruitment of migrant construction workers from this area was largely done by agents/contractors. They provide the labourers a cash advance to help the family left behind in the absence of the migrant. The advance is also used by the migrant to purchase essentials for the journey. The advances are repaid through migrant wages and the length of time that this takes depends on the payment that the migrant receives at the destination. The contractors recruit migrants in groups who stay together at the destination. Living conditions at construction sites and working place of the migrant s are appalling

and contractors provide only the most basic shelter. Harassment by the police, urban authorities and contractors is common to the Migrant Bhumijwomen.

Findings: In the light of Objective 3: To perceive the perception of the Bhumijs about the impact of urbanization. (Use of PRA tools)

Health hygiene and immunization: Those who left Lowakui10 (ten) years ago, they did not have any idea about health and hygiene. They were illiterate. Hence, they were not concern about the issue. On the other hand, the dwellers of the village were habituated in open air defecation. Government built some sanitary latrine. But it seemed to cast pearls before swine. Actually they were not sensitized. They did not feel the necessity of sanitary latrine. Education has knocked on the door of the casual labours of the cities. It is because of urbanization. As they live at the industrial belt, they have enough opportunity to be sensitized regarding the issue. The NGOs often organize motivation camp on the necessity of sanitary habits (in city slums).

Declining food insecurity: 78% respondents of the migrant and only 8% respondents of non migrant are food secure. 16% respondents of migrant and 40% of non migrant are food insecure without hunger'. 6% respondents of migrant and 40% of non migrant are Food insecure with moderate hunger'. But there is no respondent who is food insecure with severe hunger 'atmigrant. 12% respondents of non migrant are food insecure with severe hunger'. (United States Department of Agriculture's food security scale, 2000 is used).Migrant is nearer toPurulia, Assansol, Bokaro and Tatanagar. Most of them have paid income source. Hence, they have access to secure foods. But the dwellers of the non migrant survived as best they could on a bit of rice each day plus somechakora, a spinach-like vegetable, and the roots of a plant known as *gethi*.(The problem is that *gethi*is poisonous. It needs to be soaked in water for 24 to 48 hours to leach out the toxins and become safe to eat).They also survive on food gathering and hunting. But they have not any safe subsistence economy. So to say these inverse conditions stimulate their food insecurity.

Educational aspiration for the children: 2% parents (among the migrants)have desired to provide secondary education to their children. 8% mothers would like to provide higher secondary education to their children.30% mothers would like to see their children as graduate. 36% mothers have aspiration to send their children in university. 24% mothers would try to provide technical education to their children. They claimed that they were exploited in the city as they were not educated. Some of them were unable to calculate also. They did not want that their children would exploit like them. Social security here played a vital role. Hence, they decided to make their children educate so that they could enjoy a better future.

CONCLUSION

The findings prove that the urbanization has dual impact on the lives ofBhumijs.Those who live nearer to the industry/ urban belts they have the problem of detribalization. On theother hand, the non migrantdwellers ofLowakuihave separate problems. They are economicallybackward. **12% of them are „Food insecure with severe** hunger.Migration becomes a common issue in post urbanization period. While thetribes are migrating in the industrial belt i.e.Assansol, Bokaro, Tatanagar, in that time their family facedtremendous blow of poverty. Finally it can be concluded that those who are living nearerto the city, became economically sound than those of who reside away from the city. But detribalization grasped their culture. They lost their self identities. Hence, itcould be concluded that the development should be for the tribes, of the tribes and bythe tribes.Swain (2009) commented on this issue: These people are asking verypertinent questions; why should they be obliged to endure disproportionate costs ofdevelopment and why in the process of development should they be treated as lessercitizens? These questions are all the more relevant when viewed from theConstitutional vantage point. The preamble of the Constitution of India, speaks ofjustice, social, economic and political, and the Constitutional spirit, is arguablyespoused by Article 14 which guarantees *equality before law* and *equal protection oflaws*.

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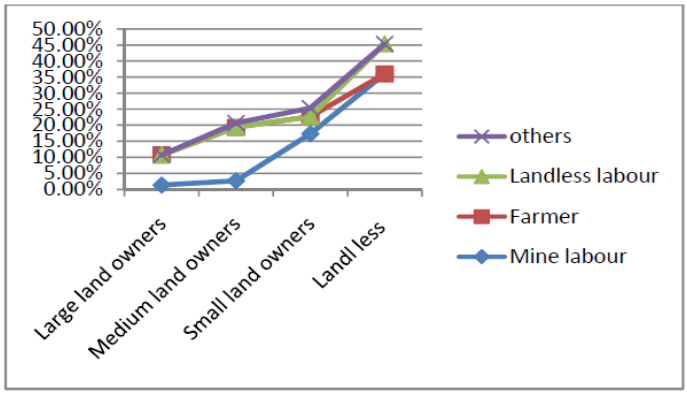

Figure:1 Relationship between land ownership and occupation

Table1: Relationship between ownership of land and occupation

Chi-Square Tests						
	Value	Df	Asymp. Sig. (2-sided)	Exact Sig. (2-sided)	Exact Sig. (1-sided)	Point Probability
Pearson Chi-Square	54.334[a]	9	.000	.000		
Likelihood Ratio	64.012	9	.000	.000		
Fisher's Exact Test	53.122			.000		
Linear-by-Linear Association	4.989[b]	1	.026	.028	.017	005
N of Valid Cases	75					

Table 2: Relationship between urbanization and traditional folk culture (Chi-Squire Test)

Chi-Square Tests					
	Value	Df	Asymp. Sig. (2-sided)	Exact Sig. (2-sided)	Exact Sig. (1-sided)
Pearson Chi-Square	5 8.594[a]	1	.000		
Continuity Correction[b]	5 4.753	1	.000		
Likelihood Ratio	6 6.919	1	.000		
Fisher's Exact Test				.000	.000
Linear-by-Linear Association	5 7.812	1	.000		
N of Valid Cases[b]	7 5				

a. 0 cells (.0%) have expected count less than 5. The minimum expected count is 9.00.

b. Computed only for a 2x2 table

Table 3: Impact of urbanization on the income of the respondents living nearer from the urban area

t-Test: Paired Two Sample for Means

	Variable 1	*Variable 2*
Mean	746.5833333	1203
Variance	271078.4275	648776.2609
Observations	24	24
Pearson Correlation	0.956701835	
Hypothesized Mean Difference	0	
Df	23	
t Stat	-6.524816054	
P(T<=t) one-tail	5.85702E-07	
t Critical one-tail	1.713871517	
P(T<=t) two-tail	1.1714E-06	
t Critical two-tail	2.0686 57599	

Table 4: Impact of industrialization on the income of the respondents living away from the industry

	Variable 1	*Variable 2*
Mean	529.2	206.4
Variance	226156.7	34487.3
Observations	5	5
Pearson Correlation	0.974720365	
Hypothesized Mean Difference	0	
Df	4	
t Stat	2.426598555	
P(T<=t) one-tail	0.036122957	
t Critical one-tail	2.131846782	
P(T<=t) two-tail	0.072245914	
t Critical two-tail	2.776445105	

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REVIEW ARTICLE

Digital Financial Inclusion: A Review

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ABSTRACT

Present paper describes various facts and facets of digital financial inclusion. In order to increase customers and also to approach more people in digital financial services and DFI has been developed for making it more economically stable for the customers belonging to different economical background. Along with several benefit that has been possible after digital financial services came into existence, there are some challenges arose too. In 12th Mint Annual Banking Conclave the Deputy Governor of Reserve Bank of India, N.S. Viswanathan said that, "Digital Platform of financial services improved the financial inclusion; it has not only benefits the customers but also improved the credit assessment for the lenders. Present paper could be considered as a tool to analyse DFI. The paper is concluded with a remark: It can also be said that, Digital Platforms are majorly facilitates urban people rather than rural people. Although urban people are also facing several challenges to be a part of digital financial services, like generation gap is a major issue for understanding digitisation of financial services.

Keywords: DFI, Digital Platform, e-commerce, financial inclusion, RBI

INTRODUCTION

Digital Financial Inclusion is an initiative to reaching out more customers and people who are already using bank and such formal financial services, and make formal finances more accessible and affordable to them. The innovation of digital financial services make millions of people moved to cash based transaction to formal financial services. In order to increase customers and approach more people digital financial services has been developed for making it more economically stable for the customers belonging to different economical background. Along with several

benefit that has been possible after digital financial services came into existence, there are some challenges arose too. In 12th Mint Annual Banking Conclave the Deputy Governor of Reserve Bank of India, N.S. Viswanathan said that, "Digital Platform of financial services improved the financial inclusion; it has not only benefits the customers but also improved the credit assessment for the lenders. Among the lenders the segment of digital financial services benefits self-employed, small and micro enterprises and small borrowers as well who are considered to be inefficient for the formal financial services."

Digital Financial Inclusion can be defined as increasing and improving financial accessibility and increasing usage of formal financial services for the *financially excluded and the undeserved people,* in terms of making it possible the digital platform had been developed to be user's friendly and improved financial accessibility and economic stability which suits both the consumer and provider. In simpler words, Digital Financial Inclusion can be defined as a digital platform where people can make payments, do transactions. It also facilitate the *financially excluded and financially undeserved people* by saving, lending, insurance and providing economic security as well.

Inside into the DFI: In the 12th Mint Annual Banking Conclave the Deputy Governor of Reserve Bank of India, N.S. Viswanathan also said that, "it has been predicted to reach about 284 billion USD in 2016 from 11 billion USD in 2013." He added to his point that, "a analysis has been directed by the Boston Consulting Group who had assessed the growth of digital financial services and observed an exponential progress in next few years.

A study has conducted on UPI money transactions, which shows that, there is a jump of transaction of almost 18% against February, 2019, whereas there is a jump of 25% amount transferred through digital platform which is the highest jump in last few months.

According to National Payment Corporation of India, they revealed a data of Immediate Payment System (IMPS) that, in March 2019, 190 million transactions has been completed in whereas 166 million transaction has been done through Immediate Payment System (IMPS) which is 14% jump of number of transactions in one month. They have also been added that, the total transaction amount is nearly 1.7 lakh crore, comparing to this; the total transaction amount is almost 1.5 lakh crore.

National Payment Corporation of India has also revealed that, there are also many digital platforms where online transactions has been done, such as National Electronic Toll Collection, which is a digital transaction platform where the payment is being done without stopping at any toll. In National Electronic Toll Collection there is a shift of online transaction of nearly 2.2 million in March as compare to February, 2019.

Data trends: A discussion: The above data and trends are showing the enormous use of digital transaction over the period of time. The number of transaction and amount of transaction is increasing day by day, so it can be assumed that people are getting more involved in digitisation of transactions and people are becoming more aware about digital transactions. The facilities the customers are getting and the benefits digital finances are providing is the consequence of rapid growth of digital financial services. In Mint Annual Banking Conclave DilipAsbe, Managing Director and Chief Executive Officer of the National Payments Corporation of India (NPCI) talking about future of Digital Financial Services in India that, "in a country like India where cash-based transaction is popular than other transactions, in that time digitisation of financial services are in a critical period which will remain few more years, people need to be digitally educated, which requires few time."

The trends and the upliftment of Digital Financial Services are clearly showing that there are numerous advantages for using digital financial services. There are several thing which are being upgraded by Center for Digital Financial Inclusion in digital Financial Services. Some of the notable advantages which help customers and motivate to use Digital Financial Services are as follows,

Digital empowerment of citizen is one of the main center of attraction among the several other advantages. Along with the traditional financial knowledge, there need to be awareness of digital platforms of financial services. So the rapid digitisation of financial services is providing empowerment to the people.

There is no such long queue in digital transaction, and one tap transaction, money transfer is possible now. Which saves time of the people rather than waiting in a long queue in bank and other financial institutions? Other than that, people needs travelling cost in traditional financial services whereas digitisation of financial services saves money for that. Along with that digital transactions have easier transaction process and payment methods.

Digitisation of financial services does not need enough documents which is very helpful to the rural poor having less formal document, for which a major proportion of rural poor is being excluded from formal financial services, but digital financial services they are not excluded from banking and financial services.

Digital Financial services are available 24X7 which helps people in any time transaction at any place around the globe. Some digital platforms like NEFT (National Electronic Fund Transfer) and RTGS (Real Time Gross Settlement) are so popular now day, due to low cost transactions and money transfers and it is also one of the fastest modes of money transfer.

Traditional method of financial services requires much paperwork which is not eco-friendly, in case of digital banking there is no such paperwork required so the digitisation of financial services is environment friendly.

Disadvantages

Like numerous benefits and advantages, there are also some disadvantages too which does not let the Digitisation of financial services meet the main objective to meet the *financially excluded and undeserved people.* Although it has a great achievement in online transactions, Digital Financial Services failed to reach the poorest of the poor.

The main disadvantage that begins with digitisation of financial services is literacy and digital literacy among the users of digital platforms. In case of interior parts of rural India, there are numerous uneducated people who don't even able to read alphabets, rather than that, digital financial services required the knowledge of using devices used in digital finances. So, it is quite getting failed to achieve reaching the people of interior parts of rural India.

Awareness of Digital financial services is one of the essential things to use digital finances; there are plentiful people who are still unaware about digital finance which makes them excluded from digital finances.

As mentioned above interior parts of rural India is still lacking in electricity and network availability, so there is no chance to build up a system of digital financial services.

There are people in India who can hardly afford two times food for their family, for them affordability of digital devices is quite impossible; hence financial using digital financial services by them is always will be question.

There is a requirement of hard cash in everyday life especially for the traders, so all time digital finance using is impossible for everyone.

In 21st digital security is a big question mark. There is no security for online transaction and online payments though the digital finance providers are trusted. There are several cybercrimes are happening all around the globe. So there always will be a security issue for the digital financial services.

CONCLUSION

In case of if rural India is ready or not for Digital Financial Services, there are several advantages and demerits for using digital platforms. Electricity and network coverage will always be an issue for mobile banking but many network providers are trying to increase their coverage area which may help the rural part of the country. *Textual and technical literacy* will always be a problem but awareness campaigns are a probable solution to overcome this. But Digital Financial Services are also helpful where using alternative financial services and accessing formal financial services is a great challenge.

In a concluding part, it can be said that, digital financial services are more successful among urban poor rather than the rural poor and the poorest of the poor in India. It can also be said that, Digital Platforms are majorly facilitates

urban people rather than rural people. Although urban people are also facing several challenges to be a part of digital financial services, like generation gap is a major issue for understanding digitisation of financial services.

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RESEARCH ARTICLE

Conceptualizing Minimum Support Price in Agriculture

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ABSTRACT

The minimum support price which is fixed by the CACP, actually considers the factors regarding the production function. It includes the cost of production at different levels which consists of costs of inputs such as seed, fertilizer, manual labour as well as machineries and also entails the implied cost of family labour and in the final stage includes the implied rent on land and interest on capital assets. The procurement price is the price which is usually higher than the minimum support price but not have any connection with open market price. The MSP is the very important for the product which are covered under it. But it has also some demerits. The small and marginal farmer can't get the full benefit from the MSP. The big farmer only gets the benefits. MSP and Procurement price both are fixed by Government and maintain by Government only. The open market doesn't have any relation with it. Government has its some procedure to collect the procedure and the payment also not done immediately. The small and marginal farmer who needs the immediate cash can't wait for government procedure. Present article focuses on various facts and facets of MSP.

Keywords: MSP, CACP, Cabinet Committee of Economic Affairs, National Agriculture Cooperative Marketing Federation of India Ltd.

INTRODUCTION

Minimum Support Price (MSP) is a form of market arbitration by the Government of India for Agriculture Produce. The minimum support prices are declared by the Government at the beginning of the every sowing season of Particular crop for specific yields based on the suggestions of the Commission for Agricultural Costs and Prices

(CACP). MSP is the price which is an assumption done at the beginning of Crop Season. MSP is the backbone of our countries Agriculture. Farmers get their faith to have some profit by cultivating the crop. MSP helps them to quantify the area of cultivating and the amount they should put for Farming this year. MSP price is determined by Government and maintain by Government only. The market price may be differing from the Minimum Support Price. MSP is not applied for all the crops. It is only applied for 25 crops from largely cereals, pulses and oil crops. The crops which are perishable don't come under Minimum Support Price. The crops which can store easily and have a huge use are come under MSP.

The MSP is fixed with the idea is that the crops price can't go down to this level in any condition like huge Production. Government also issued Procurement price for the crop which comes under MSP. The Procurement price is determined after the harvesting of the Crop. Procurement is declared with the idea to give the Farmer more and more benefit from their produce. Different public agencies like Food Corporation of India procured the food grains of Kharif and Rabi season at the procurement price for the distribution through Public Distribution System. The procurement price is the price which is usually higher than the minimum support price but not have any connection with open market price.

Historical Perspective

The minimum support price fixed by the CACP by considering the factors regarding the production function. It includes the cost of production at different levels which consists of costs of inputs such as seed, fertilizer, manual labour as well as machineries and also entails the implied cost of family labour and in the final stage includes the implied rent on land and interest on capital assets.

In 1965, first MSP was declared by Government of India. From then till now it plays a significant role. The Cabinet Committee of Economic Affairs (CCEA), Government of India, fix the Minimum Support Price. It is fixed as a National Level with the help of Commission for Agricultural Cost and Prices. But to fix the National level MSP it has to play a very significant role of every State Government to find out the input cost of every crop. To find out the Input cost the state has some tier wise structure as village household level to district level. Sometimes any Non-Governmental Agencies may also involve in this process.

Inside into MSP

In this country due to diversified agro-climatic condition the crop varies from state to state. Generally the crops sown in Kharif and Rabi season come under minimum support price policy. The Government of India and CACP selected 25 general crops including Paddy, Jowar, Ragi, Bajra, Maize, Arhar, Moong etc as Kharif Crop; Wheat, Barley, Gram, Masur etc as Rabi Crop; Cocunut, Jute, Sugarcane etc.

Specific case

The state like West Bengal we can only found Jute and Rice are the Major crop which is covered under MSP. Despite of huge no of crop which has a very good production in West Bengal but only this two crops are procured. The State Government's Food and Supplies Department is responsible for the Procurement process of crops. In every district there are Directors to manage the whole process. The procured food grains are used for Buffer Stock and Supply through the Public Distribution System. For Rice we can found a state level structure but for Jute we can't find a state level structure in West Bengal according to Niti Ayog Report (2016). For Rice in West Bengal the MSP is operates through three agencies i.e. National Agriculture Cooperative Marketing Federation of India Ltd. (NAFED), National Cooperative consumers Federation of India Ltd. (NCCF), West Bengal Essential Commodities Supply Corporation Ltd. (WBECSC).

The MSP is the very important for the product which are covered under it. But it has also some demerits. The small and marginal farmer can't get the full benefit from the MSP. The big farmers only get the benefits. MSP and Procurement price both are fixed by Government and maintain by Government only. The open market doesn't have

any relation with it. Government has its some procedure to collect the procedure and the payment also not done immediately. The small and marginal farmers who need the immediate cash can't wait for government procedure. Some issues related to MSP are like, Farmer focused on those crop which has high MSP and Covered under MSP; all farmer want to sell their product to Government, it may leads to shortage of product in open market; the MSP is fixed by an assumption and seeing the previous year's trend, the survey for MSP sometimes goes wrong which may lead to an bad assumption of MSP; the produce which is not cover under MSP but has some good value at regional basis sometime face huge loss; the access of MSP is not equal, sometime MSP stays below open market rate, then it becomes problem to Government to gather product; the payment procedure of MSP to the farmer is very lengthy etc. These are some issues and challenges related to MSP have to face by the people.

The increasing in MSP of agricultural production hastens the process of accumulation. However, the small and marginal farmers are generation small amount of surplus and that surplus they are selling in the local market. The small and marginal farmers are producing less amount of surplus product and this surplus product need to be market with MSP. The rural rich who are also produce surplus producer and they have good transport facility and they will get benefit from the MSP but most of the small and marginal farmers are not able to sell there product in the government market. They totally depend on the local market and which is not covered by MSP. The farmer will get MSP price for their product only in the government market. The sometimes the farmers are selling their product in the local market through the local agencies with the prices and that price more than minimum support price. Most of the small and marginal farmer in rural areas they sell their surplus product due to the needfor immediate cash. Therefore, the increasing MSP of the agricultural commodities will leads to increase of final products of the industry as they used formal row material. As a result, the poor small and marginal farmer will get more affect due to increasing expenditure on food and another living cost. Therefore, increasing MSP will not help small and marginal farmers.

CONCLUSION

In our society has lots of diversity and inequality in terms of cast, gender, class, and religion. Therefore, it is necessary to look at another factor with increasing MSP for small and marginal farmers. It will be a better option if the government of India looks at other factors that are most important for the small and marginal farmers in India. If the government provide subsidies inputs such as fertilizer, new technology, and other input then they will increase profitability from the crop production. There is no good road, and transport facility in rural areas. The largely small and marginal farmers do not have good irrigation facility and other infrastructure that is most important for the farmers. Therefore, the government should more investment in this infrastructure. These are the fact that more important than MSP. The government agency should have reached the village level and increasing market linkage in the rural areas so that farmers can sell their product direct to the government. One of the most important things is that most of the rural farmers are not aware of the MSP for their product and they are totally depending on an intermediarytoselling their product. Therefore, the government should element this intermediary and government agency should reach the village level and purchase their product. The information should be provide at the village level. The government market should link with the village market then the small and marginal farmer will get benefit from the MSP.

The current government of West Bengal is doing a campaign at the village level for the purchase of agricultural commodities direct from the farmers. Due to this intervention, the farmers can sell their product direct to the government at the procurement price. The farmers are not depending on an intermediaryto sell their product. This intervention happened at the three levels such as Block, Panchayat, and village level. The farmers get money by checks from the government office like farm or Panchayat office. This intervention reduces farmers transport cost and the role of intermediary. The choice of crop for MSP should be based on regional each season. Therefore, the region farmers will get MSP on their regional crop. These interventions start this year and they collect rice at the procurement price. The whole campaigns managed by the local agricultural produce market committee.

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RESEARCH ARTICLE

Institutional Linkage Fitches Farm Sustainability: a Specific Case of Family Farming

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ABSTRACT

For centuries, tribes of the 'Chotanagpur Plateau' region have stayed in geographical isolation, have maintained their distinctive culture of farming, have sustained on family farms, and struggled to overcome poor socio-economic condition. The tribal groups of this region have stayed outside the realm of the developmental outputs because they reside in forests and hilly tracts. On the other hand, the plateau of Jharkhand is popular for its mineral resources. Industries often consider these people as the passive resources. They have been used as cheap labour forces. As a result, several NGOs with their novel approaches, use to help people. Present study is an output of ex-post facto research design. Network Analysis is an integral part of it. The study concentrated on a specific case which revealed the family cases of East Singhbhum, Jharkhand. Finally, it concluded with a remark: Farm size had positive significant correlation with food security because bigger the farm size more would be the resources of the family with more viability which will naturally lead to increase in food security. Contact with NGOs too had positive significant correlation with food security which indicated that the relation with NGOs would help them to raise their capacity through training, information and sensitization. It may be because the village dwellers, associated with NGOs had good access to information or may be because they were aware of the new technical and farm related information which was given by these sources.

Keywords: Family Farming, NGO, Network, Case Study, East Singhbhum

INTRODUCTION

Chitambar (2015) defined 'Social Organization' as the classes of human relationship structures wherein individuals intentionally related in methodically orchestrated units to advance and accomplish some normal purposes or interests that are not particularly communicated in the establishment. In association every part has a formal status and part. It might be characterized as a gathering with unique concern and interests that have built up a structure including particular parts for different individuals, and that have a pretty much formal arrangement of guidelines and directions for operation. An association varies from an establishment by its attention on a barely restricted reason. It is gathering of individuals sorted out to seek after particular goals. Association may work inside organization. But the concept of 'institution' is quite different. Horton (1964) opined that institution is an organized arrangement of social connections which epitomizes certain regular qualities and strategies and meets certain fundamental needs of society.For centuries, tribes of the 'Chotanagpur Plateau' region have stayed in geographical isolation, have maintained their distinctive culture of farming, have sustained on family farms, and struggled to overcome poor socio-economic condition. The tribal groups of this region have stayed outside the realm of the developmental outputs because they reside in forests and hilly tracts. On the other hand, the plateau of Jharkhand is popular for its mineral resources. Industries often consider these people as the passive resources. They have been used as cheap labour forces. As a result, several NGOs with their novel approaches, use to help people. Present study concentrates on a specific case of a family farmer.

Objective

To trace out the networking of a family farmer

MATERIALS AND METHODS

The study was conducted taking samples from the East Singhbhum district of Jharkhand State. Multistage sampling technique was adopted for the selection of study area and sample respondents for collection of information required for the study.

Findings: A case study

'Since 12 years I have been thinning out innovative 'low cost technologies strategy' subsequent to creating links with various Government as well as Non-Government Organization (not only the organizations, working at my native place, but also with the organizations of other states). I attended several training programmes…..There was no government support for spread of new farming techniques aside from a couple of NGOs had some supporting initiative.

Simanta Mishra

Simanta Mishra, of Dhatkididh village, Patamda He was a progressive farmer. Age is about 35 years, B.Sc. passed. Their family was migrated from Odisha and started agriculture in that area in about 1940. They were the land lords or *Zamindar*of that area. He was very much fond of diversified production. He ranked first in respect of resource integration in his farm. Wellbeing ranking revealed that he was the most 'Resource Rich' farmer of the area. His farm was very much productive and the other neighbour farmers were following him, adopt modern technologies. It was revealed from the FGD that he was the key person with whom NGOs used to contact to disseminate a new technology.

Agri-entrepreneur Simanta opined '*I have reduced the costs of agricultural production by limiting the use of chemical inputs. IFS and IPM helped me a lot. I'm in this field since last 15 years. I attended more than 18 out of state training programmes*'.

Exhibit - 1 from Specific Case

Respondents in the course of their understandings, discussed and explained the strengths of Simanta's Farm-

- Resource rich farmer
- Highly educated
- Cosmopolitan sources of information
- Risk taking ability
- Skilled and well trained farmer
- Good marketing linkage
- Knowledge about farmer centric government schemes and policies
- Good connection with NGOs, KVK, ATMA, RRS and SAU.

The information accumulated through the FGD and Sociometry gave data on the 'data rivulets' inside the group and their explanations on various sources of information and social interaction pattern of Srimanta was analysed and represented through socio-gram.

Exhibit - 2 from specific case

The institutional networks and liaison at the grassroots, if utilized properly, can act as a change maker and able to strengthen the family based farms. Capacity building of the farmers having small farms may reinforce the food security at family level and empowerment at community level.

Impact on Family Level

If properly adopted with investment in maintaining improved yields without depleting natural agriculture, IFS improves the personal savings and health resources or destabilizing the environment. Integrated farming is a commonly and broadly used word to increased food production; social function in terms of explain a more integrated approach to farming as provision of employment opportunities for excess labour compared to existing monoculture approaches.

* Significant at 5 % level of significance
** Significant at 1 % level of significance

Table 2 depicts the correlation between food security and other independent variables. It has been found that the variables Size of the farm (X_5) and Contact with NGOs (X_{12}) had recorded significant correlation with the dependent variable food security while the variables Social Interaction (X_{14}) and Good liaison with Government Organizations (X_{15}) had significant and correlation with food security.

CONCLUSION

Farm size had positive significant correlation with food security because bigger the farm size more would be the resources of the family with more viability which will naturally lead to increase in food security. Contact with NGOs too had positive significant correlation with food security which indicated that the relation with NGOs would help them to raise their capacity through training, information and sensitization. It may be because the village dwellers, associated with NGOs had good access to information or may be because they were aware of the new technical and farm related information which was given by these sources. Food security is both biological and perceptual display of calorie intake balances, interaction pattern and liaison with Government Institutions. When one was crippled with food insecurity he was supposed to run with low social interaction and connection with institutions.

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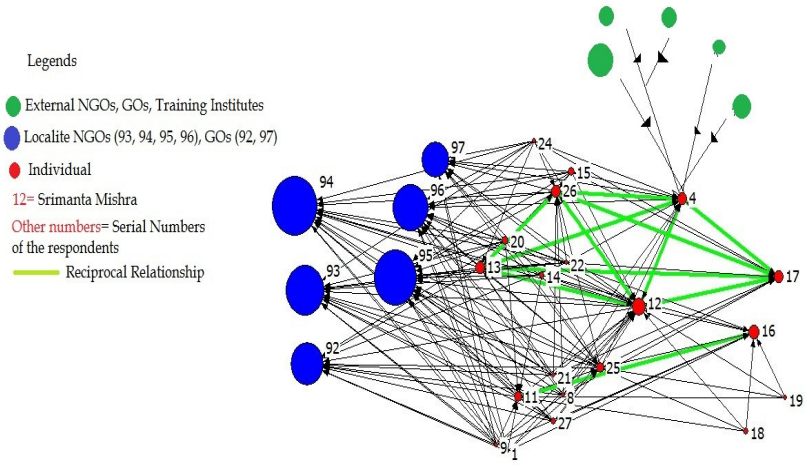

Figure 1: Socio-gram of Simanta Mishra's interaction pattern

Table 1: Selection of the study area

State	District	Blocks	Villages
Jharkhand	East Singhbhum	Ghatshila	Darisai, Bodhpur, Bhamradih
		Patamda	Dongagarh, Dhatkidih, Loraidoongri
		Bahragora	Jarabani, Pochakhuli, Satpati

Sampling: Purposive Sampling method was adopted.

Table 2: Co-efficient of Correlation: predictor variables and food security

Variables	R value	Remarks
Age	0.123	
Family Size	-0.054	
Education	0.044	
Occupation	-0.045	
Size of the farm	0.153	*
Farming Experience	0.059	
Outside Contact	0.167	
Localite Contact	0.121	
Community Cohesiveness	-0.028	
Interpersonal Source	0.021	
Leadership	-0.050	
Contact with NGOs	0.260	**
Good behaviour with naibours	0.158	
Social Interaction	0.288	*
Good liaison with Government Organizations	0.149	**

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RESEARCH ARTICLE

Community Networkingof Family Farms: Impendingluminosities on East Singhbhum, Jharkhand

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ABSTRACT

Enhanced data alone however is not adequate for enhanced basic leadership. Basic leadership is a political procedure and partner interest in basic leadership procedures is critically imperative. The SL approach is on a very basic level individuals focused and requests a point by point participatory evaluation of the qualities and data needs of target recipients and partners as an early action in program plan. This needs to connect with partners at all levels, advance two-path streams of data amongst them, and focus on the part of data in connection to various business resources. At long last, it finished up with a comment: Farm size had positive huge relationship with food security in light of the fact that greater the homestead size more would be the assets of the family with greater reasonability which will normally prompt increment in food security. The study was carried out in East Singhbhum, Jharkhand. Purposive Sampling is used here to draw the subset of population. PRA and FGD are the basic methods of data collection. Finally, the study divulges: Contact with NGOs too had positive huge connection with food security which demonstrated that the connection with NGOs would assist them with raising their ability through preparing, data and refinement. It might be on the grounds that the town tenants, related with NGOs had great access to data or might be on the grounds that they knew about the new specialized and ranch related data which was given by these sources

Keywords: FGD, PRA, Family Farming, Community Network, East Singhbhum.

INTRODUCTION

To comprehend correspondence inside a Sustainable Livelihood (SL) system eludes to, as a rule, smaller scale large scale linkage accentuation. For further elaboration, bolster from the idea of AKIS (Roling, 1988; Engel, 1995 as specified by Skerratt, 1998) can be looked for. Roling (1988) characterized a horticultural data framework (AIS) as -a framework in which rural data is created, changed, gotten and nourished back in such a way, to the point that these procedures work synergically to support information use by agrarian producersand a rural learning framework (AKS) as -a arrangement of conviction, insight, models, hypotheses, ideas and different results of the brain in which the… experience of a man or gathering regarding farming generation is accumulated. Nonetheless, notwithstanding these, one can locate a more important and official/crossing over point from one of Roling's (1985) prior distribution, where he watched that a horticultural information framework cooperates with non-agrarian learning frameworks, money related and showcasing frameworks, with approach detailing and usage frameworks, with natural frameworks et cetera. This serves two of the present interests – to begin with, demonstrates a large scale small scale linkage understanding and second, approaches towards an idea much closer to work (learning) data framework. The study intends to track down the following objectives.

a. To find out the community network of Family Farming
b. To describe the role of social interaction in Family Farms

MATERIALS AND METHODS

Locale of the study area

Present study was carried out in Paamda of East Singhbhum, Jharkhand. Expanding on the portrayals of the institutional impact which farmers perceived and explained to the present researcher during data collection, this segment examined and figured out how institutional extension activities created positive changes by helping them to move towards the sustainability of their family based farms.

Initially, the aftereffects of a three round 'FGD based power mapping' practices, entitled as 'Shared Influence Analysis', directed in farmers and institution were exhibited, demonstrating farmers' view on the said topic.

FGD based power mapping

FGD held with selected farmers from the study area in each gave important bits of knowledge into the ways farmers were impacted by their association with various institutions. FGD discourses meant to examine the degree to which farmers feel engaged to comprehend the issues they confront and the components that empower and oblige farm dwellers from reaping better result from newly emerged technologies.

FGD exercise and data analysis

- Farmers were asked to find out the positive and negative impact of institutional attachment
- Preparation of the 'influence list'
- Identification of specific cases
- Transcription of FGD data
- Analysis from transcription -> segregation of thematic elements -> words, theme, character, repetition, quotes

RESULTS

One of the main focuses of the present investigation was to trace out the relationship between the group cohesiveness of the Self Help Group. Because, result of FGDs were suggesting that NGOs had been an impact on social inclusion at community level. To find out the group cohesiveness of the Self Help Group, the present

researcher applied the technique of 'Sociometry' and for applied the mentioned technique the investigator considered the frequency as score and the relationship between the group cohesiveness of the 'Self Help Group' and the empowerment of the SHG members was find out with the help of Pearson's Product-Moment Correlation.

As the value of *r* is - 0.656787465then it can be said that there is no such relationship between the group cohesiveness of the Self Help Group and the empowerment of the SHG members.

Significance of *r* is determined directly by consulting the table values of Pearson's Product-Moment Correlation. The table value of r at 0.05 level of significance and at 8 degrees of freedom is 0.643. As the computed value of r i.e. 0.656787465is greater than the table value, then the null hypothesis was rejected and we can conclude that the group cohesiveness of the Self Help Group and the empowerment of the SHG members were significantly correlated.

Community Case

Reviving the traditional farms at Patamda: A case of community movement

The community members of Patamda were not acquainted with alley cropping. Tagore Society and TSCSR introduced here alley cropping. In this area, mostly arable crops were suitable to grow. Alley cropping exploited the viability of arable cropping system. Arable crops were introduced in various alleys formed by perennial trees, set up on contours. Trees were acted as live bunds to control run off. Locally available stones were also used for bunding and to check run off.

According to the community members of Patamda, it was a relevant step which had a great impact on their farm sustainability. Advantages in terms of linking the community members with various institutions appear apparent.

Role of institutions apparently was acknowledged by the community members especially for technology refinement and promotion. It was revealed from the FGD that since 1980, Tagore Society was working there with multi-facet approaches, which arose from an in-depth understanding about the felt needs of the community.

Exhibit - 1 from Community Case: Drawing inference

Since, present researcher intended to ventilate the impact of the institutional initiatives in the case area; present researcher collected information from 24 farm families on the difference that has occurred in the yield before and after the institutional linkage.

In order to judge whether the change in the yield was statistically significant, we have undergone a statistical test. As the two variables under study (Yield in kg/acre) were scale variables and since the study intended to depict the difference in the yields before and after the introduction of the SRI programme, researcher had undergone "t-test: Paired sample for means" in SPSS.

Since, the farmers expressed their yield in different units, so ,in order to facilitate easy calculation all these units have been converted to kg/acre.

Statistical Hypothesis

Ho : The difference in the yields(kg/acre) before and after institutional linkage is not statistically significant
H1 : The difference in the yields (kg/acre) before and after institutional linkage is statistically significant
where, H0 = Null Hypothesis
H1 = Alternative Hypothesis

Critical Value

At 0.05 level of significance and degree of freedom 23, the critical value of 't' is 2.069.

CONCLUSION

The participants themselves identified and explained the different aspects of community level empowerment. These aspects were represented through five specific arms which were observed on a five point scale, where zero represented lowest level of empowerment whereas five was depicting the highest level of empowerment. From the study it was clear that institutional linkage stimulated empowerment at community level. The visual depicted clearly that community members had a lesser empowerment level (in all aspect), before they had linkage with various institutions. Role of institutions apparently was acknowledged by the community members especially for technology refinement and promotion. It was revealed from the FGD that since 1980, Tagore Society was working there with multi-facet approaches, which arose from an in-depth understanding about the felt needs of the community.

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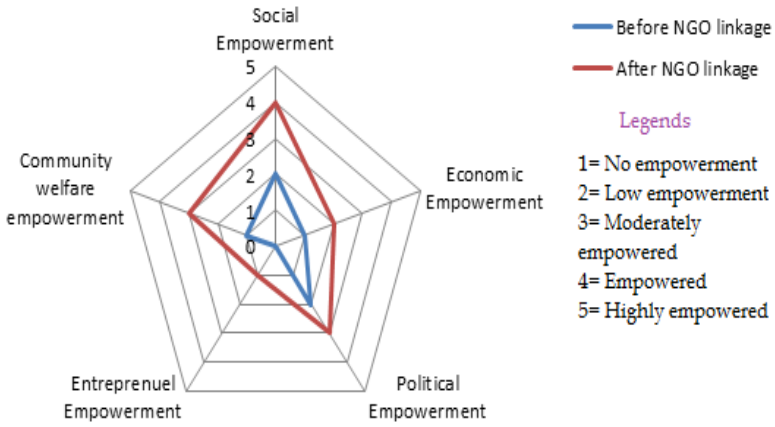

Figure 1: Community level empowerment: Rader diagram

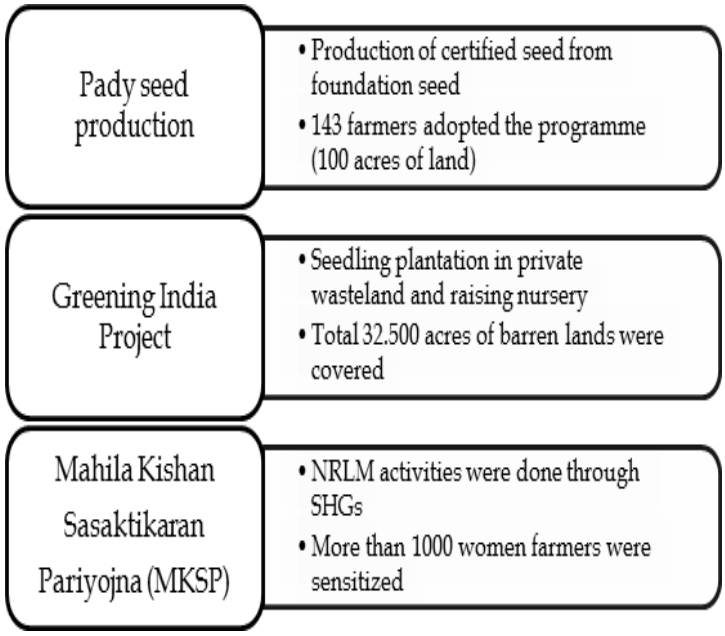

Figure 2: Impact of community based projects: A highlight

Table 1: Correlation between Group Cohesiveness and Average Score of empowerment

SHG	Group Cohesiveness	Average score
Group 1	0.1789	18.32
Group 2	0.1566	14.43
Group 3	0.1956	10.67
Group 4	0.1282	9.87
Group 5	0.1675	14.43
Group 6	0.2563	9.87
Group 7	0.2750	7.89
Group 8	0.1762	12.12
Group 9	0.1777	14.56
Group 10	0.2857	14.76
r = - 0.656787465		
Level of significance = 0.05; Degrees of freedom = 8 (N-2=10-2)		

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RESEARCH ARTICLE

Community for Livelihood Interventions: Realism and Challenges

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ABSTRACT

This work is intending to arouse an extent of controversy regarding challenges of Community organizations. Community organization or association is a valuable concern with endeavours to coordinate social assets successfully towards the particular or aggregate welfare needs any geographical zone. Its execution may include such activities as, real findings, coordination, enhancing benchmarks, understanding improvement, welfare programs, changing pattern of formative action or developmental activity and promoting social legislation. However, communities have various diversification of social ills, social issues or social problem. Through the community organization method, communities act like totality and working for irradiate the problems and bring the benefits of social welfare. Finally, the study tried to ventilate a concluding remark. It clarifies peoples' association and its impact. Consequently, people group association brings about strengthening of individuals. The strengthening encourages the group to remain against abuse, pick up the capacity to take care of issues and to accomplish the coveted objectives. A significant number of the monetary issues can be effortlessly tackled by community organization and strengthening of the community. Many times due to misbehaving of the institution the community cannot reach their goal. However, it is a participation process so the community involvement and their engagement can irradiate their problems.

Keywords: Community organization, SHG, MYRADA, FPO, Social organization

INTRODUCTION

The word 'Livelihood' can be utilized as a part of a wide range of ways. The accompanying definition catches the expansive idea of occupations comprehended here: A Livelihood contains the abilities, assets (along with both material and social assets) and action required for a means of living. A livelihood is reasonable when it can adapt to and recoup from stresses and stuns and keep up or upgrade its abilities and resources both now and later on, while not undermining the natural resource base. Livelihood is the most important part of any family as well as a community. However, the livelihood depends on five capitals i.e. physical, ecological, human, social and natural among the community. Each of the capital interlink with each other. These are the five wings of livelihood process.
Community organization or association is a valuable concern with endeavours to coordinate social assets successfully towards the particular or aggregate welfare needs any geographical zone. Its execution may include such activities as, real findings, coordination, enhancing benchmarks, understanding improvement, welfare programs, changing pattern of formative action or developmental activity and promoting social legislation. However, communities have various diversification of social ills, social issues or social problem. Through the community organization method, communities act like totality and working for irradiate the problems and bring the benefits of social welfare.

The people of community organizers built up an association with the individuals from the group which lead a review to determine the necessities and it includes the general population for the definition of plans and raising assets and executing them for the community social welfare and different administration services. The main priority of the community organization is for social welfare, whereas some scholar articulated that it should help to overcome the problem of poverty.

Through MYRADA and Market visit present researchers try to find out how a community is engaged in their own livelihood practices, on the other hand through the simulation exercise helped me to hand on experiences to the community association. Through that exercise help me to make a layout of livelihood status, participation in community organization, diversification, and different choices, risk and vulnerability etc. It also helps me to find out the role of the institution to the community organization and their livelihood interventions.

Livelihood Status

Through the real situation (MYRADA and Market Visit) we found that the poor peoples are circulated in between the trap of poverty. It also feels in simulation activity how a poor household copes up with the poverty trap. The poverty trap is act like low income gets low savings among the household and the investment amount also be decreased. As a result of their production rate also become decreased. The same picture is also visible in MYRADA field trip. The villagers have low assets or capital, so the chain of poverty trap exists. Though there is agriculture dominated livelihood lots of diversification in livelihood exist surrounding the villages. However, in the market visit, we found that those who have a small business, the earning capacity also very low but on another hand, big wholesaler or retailer have enough physical support to sustain their livelihood. Not only that they also have the strong social capital or social network, which helps them to gain maximum information as well as social benefit.

On other hand, gender role is also very important to livelihood. Ross & Sawhill (1977) said that in fact, a family is an economic unit and the family is a combination of male and female. They have equal chance to take a decision. They also said that to empower women or higher education of women in the family gives the result as economic improvement, it helps to improve the family status. If a family both husband and wife act as earning member then the family can be more sustain rather than one hand family member. Cheryl (2013) argued that there is a lot of evidence which addresses that women's bargaining power affect the developmental outcomes. There are many central advancement results which really depend on women's capacity or bargaining power to arrange ideal intra-household allotments of assets. So, women participation in livelihood is activity the most important factor. Similarly practically it also overlaps in the simulation exercise. Once the families have low capital (mainly physical) and they

do not invest more in the production model. As a result, the output came very low and for surveillance, they sold their land which means or it indicates that they fall into the poverty trap. Similarly, in the marketing chain, the middlemen create price differences among various commodities and its result directly affected to the producer and consumer. Beyond the field visit and market visit, it was found that those who have strong capital are more sustainable than the poor, who have less capital. So, each of the capital is important to create sustainable livelihood for community. So we can say that the rural livelihood is not just only poor income but also different diversification approaches. So we can say that the risk and vulnerability of any community same and it can be solved through the community organization.

Risk & Vulnerability

Risk and vulnerability or hazards have been restored as key highlights of rural economy or livelihood and poverty, and areas of now a concentration on policy or intervention (Stephen 2001). The poor themselves attempt to oversee vulnerability utilizing an assortment of ex-ante and ex-post hazard administration techniques, and through community supportive networks, yet these are both delicate and financially harming. Practically I also have seen the risk and vulnerability among the poor one. It could be ecological, geographical and also human creation risk. According to Kepe et al. (2004) and Wang et al. (2011), the connection between ecological conservation and poverty reduction has been the subject of intense debate among academics and practitioners for decades, to overcome these two inconsistent goals, both far and far away from reach. Water scarcity is the main problem of the village situation. In term of community organization risk and vulnerability is an important element for community development. However in community organization community as a client and they have the power to take the decision. So to cope up with the risk, communityitselfplays as a core element of the function. If we look up the MYRADA's intervention about water scarcity, water reservation facility can help to better irrigation facility and complement the drinking water purpose. Here the problem is about the whole village and it solved through community organization method. Similarly, the actual price of the commodity, market facility intervention can be done by the FPO; as a community organization.

Community organization as a participation action

Participation is defined as a collective action through certain process or decision making journey and it brings change or progress in developmental activity. On another hand, it community organization introduces itself as a collective action of the certain people. It helps to address the issues and realize and keep up alteration amongst requirements and assets in a community. So it is true that helping individuals viable to work with their issues and plan to understand their targets by helping them to create, reinforce, and keep up characteristics of the investment, self-course, and participation among each other and that is very difficult to manage each individual choice. Through that process, it brings a change among the community and individual relationship. As a result, it can distribute the decision making the power of the community members. Through the participation of SHG members can change their rational thinking. Now the members of the SHG members are financially viable and they can take decision among the individual and family level. Similarly, through the participation model community can make a political platform and enrich their decision making power as well as solve their common problem. So we can also say that community organization is a kind of problem-solving method, where the community people participate such kind of community development activities and reached at last their own goal. As an example we found in Russell market each of the specific commodities like tomato, fish, mutton market have their own committee, who have the responsibility to look up their market system and they have own problem, own issues, so the intervention should be perfect if their participation as well. So community organization is a collective process where the problem was solved by themselves participation and their activity.

Role of the institution in community organization

To organize any community, institution play very important role. The institution could be the government organization, non-governmental organization or other institution like SHG, JLG, and FPO etc. Generally, that kind of

organization makes a platform where a certain group of people can interact with each other and organized themselves. It could also very helpful in term of consumer awareness. As an example in Russell market we found that the association or body of the fish, mutton market helps to spread awareness (in term of market information i.e. price, quality, space, quantity) among the consumers and the seller. Similarly, MYRADA also working to the organized community and with no involvement of commercial activity, they try to intervene among their livelihood. They also make SHG for the women and organized themselves. Again come back to the water scarcity problem; the organization tries to gather the community people and intervene among them. Here MYRADA as a supportive agency who try to build up community organization and spread awareness among them. Thus we can say that institution is a very important factor for community organization.

Barriers of community organization

Generally, the poor and vulnerable people fell that they have no power. So they do not present them as a leader. But through the community organization, they feel they have the power to take decision among themselves. It develops their capacity and confidence, so they can solve their own problems. Though the community organization helps to empower them there is a lack of term of illiteracy, superstitions, caste division etc. It will take time to achieve the goal but the community people may have not sufficient time to engage with that. As a result, it becomes failure. Many times empowerment also act like a barrier, if some of the members are getting more benefit then they think they arepowerful; as a result, they exploit others and create violence. On the hand when individuals have organized themselves, they get the power. There are pioneers in the group and in the event that they are joined together, they can cooperate, and they can arrange with each other. This influences them to feel intense. Consequently, people group association brings about strengthening of individuals. The strengthening encourages the group to remain against abuse, pick up the capacity to take care of issues and to accomplish the coveted objectives. A significant number of the monetary issues can be effortlessly tackled by community organization and strengthening of the community. Many times due to misbehaving of the institution the community cannot reach their goal. However, it is a participation process so the community involvement and their engagement can irradiate their problems.

CONCLUSION

Community organization is a kind of space where the where the people come and organized themselves to fulfill their own goal. Simulation exercise helps to understand how and when the community organized. On another hand the MYRADA visit helps to visualize it. The local people organized and work with that, women's SHG made before 30; 20; 15 years etc. ago to solve their own problem. However, the market visit helps to understand through the community organization they can make a sustainable market where a people can access the resources. Families and groups join together and form communities. While working with communities we have to work with individuals, families, and groups.

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RESEARCH ARTICLE

Climate Change and Its Political Manifestation: A Terrible Issue for Sundarban Forest

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ABSTRACT

Fishing, crab collection, honey collection and other NTFP collection is the main livelihood of Sundarban region. Lots of spices among the plants and animals disappear due to climate change. Previously there was only fear of animal but now local people have less access to natural resources. Presently, without consulting with local people the industrial community started accessing the forest with support of Govt. Therefore it shapes like violence among the Govt. and the local community people. Thus the political issue display in forest and the local community. Through Joint Forest Management (JFM) Govt. of India try to conserve the ecological system of the forest without hampering livelihood of the local people. The most challenging thing is that though JFM is a bottom-up approach, in practices it does not co-exist. Therefore we need to develop a well-designed management process to make extension services accessible to the local people.

Keywords: NTFP, JFM, Forest Resources, Sundarban, Fishermen.

INTRODUCTION

The Sundarban forest, world largest mangrove forest is about 10000 sq. km. spread over India and Bangladesh country. Over the total area of Sundarban forest, approx. 40% have in India. History says that due the small river and

the floating clay made this forest around six decade. Almost 334 species of flora and 450 species of fauna are stay this huge mangrove forest. People have made relationships with this forest for life and livelihood. Fishing, crab collection, honey collection and other NTFP collection is the main livelihood of that region. As a supplementary they also do agriculture in only one season of the total calendar year. However many environmentalist and scholar articulated that with climate change, mangrove forest bears degradation process of her bio-diversity due to human disturbance, industrial pollution etc. Lots of spices among the plants and animals disappear due to climate change. The main reason behind the climate change is decreased inflow of fresh water. As a result the salinity of that region increased and affects the agricultural land as well as forest plantation and the water bodies. Therefore the livelihood of local people affected and they become fall into the poverty trap. Continuation of this procedure in light of environmental change and sea level ascent represents a terrible truth to the carbon sequestration potential and other biological community system of this mangrove forest system in future. So the environmentalist or the researcher identified that due to climate change across the Sundarban forest the degradation process started as a result the productivity and the capacity of the forest and the land capacity also decreased. It also observed that the salinity proportion of the land and the water increased. However if we look up their livelihood pattern, discussed that the main livelihood of that region is fishing. They have the absence of ecological mindfulness and furthermore the word related dangers identified with their profession. It has been identified that fish production due to ecological performance and the occupation process highly risky. They should be ever aware of the earning risks and follow regulations and legislation adopted regionally or nationally. The occupational dangers, wellbeing nerves, and dangers to the strength of the fishermen are built of the sorts of operation, the size of generation and the particular types of intrigue. A major challenge is that unsustainable harvesting may increase to the riverine like fishes, crab, and prawn gathering. The accumulation of wellbeing of the community affected so far. As an excuse the Govt. also introduce that due to human intervention the tiger population affected. But the idea was constructed by the state and the battle is constructed by artificially to reduction access of the forest, create more right over forest and exploit them. However in term of right the local community have equal right over the forest but without compromising or without consulting with local people the industrial community access the forest with support of Govt. So that it create compensatory afforestation bill among them. Therefore it shapes like violence among the Govt. and the local community people. Thus the political issue display in forest and the local community.

Chowdhury et.al.(2008) find out that every fish or crab collection trip on the deep forest water ways have very risky and dangerous due to the tiger and crocodile offensive. As a result until the fisherman came back from the forest region their spouse praying to their Good, believes over their customs and worship lake fasting, putting the vermilion tidy on their appealing God. Therefore their livelihood and their lifestyle belong to high insecurity both social and ecological pathway. However, it was told that they were not only depending on fisheries but also they collect the NTFPs from the mangrove forest for their livelihood sustainability.

Singh et.al. (2010) pointed out that although they are engaging with fish collection but they also depend over the NTFPs (especially honey). Now the remarkable thing is that total livelihood system is based on the commonplace but due to presser of climate adaptability, the total community's livelihood faced same and terrible threats. Before that only wild animal fear was the main problem among them but now they also faced lot of threats in term of natural resource accessibility.

Findings

- Increasing salinity of water body leads affect to the water body's fauna (mainly fish and crab). So the production of fish or crab also decreased.
- It effects the honey production, medicinal plant and other non-timber product also.
- State becomes more challenging factor to accessing the NTFP.
- Either they have to use the forest as unsustainable way or they leave their traditional livelihood.
- Migration of villagers to city area and worked as informal labour.

Government Initiative

After introducing Joint Forest Management (JFM) Govt. try to intervene among that kind of political situation with the local people. Through JFM Govt. of India try to conserve the ecological system of the forest without hampering livelihood of the local people. However, the most challenging thing is that though JFM is a bottom-up approach, in practices it does not co-exist. There is an unstructured top-down system present in this scenario.

CONCLUSION

There is a least evidences that can be prove that the local people get their right over the forest. To provide various kind of information, extension services now need to take into account differing data and administration needs of the vulnerable group and extension institutions need to spread service more efficiently. This frequently needs institutional rebuilding at various levels of the extension services. Some precaution about conservation of forest leading with local people, environment degradationcan be reduced. Beside that we must look up over the external stockholders intervention. To conclude if we look up the overall summary it shows that the climate change leads environment degradation and therefore it create political issue among the local community and state. There has been broad affirmation of the way that conventional state laws on conservation zone protection can represent a danger to the standard aggregate privileges of neighborhood groups possessing these zones, instigating livelihood vulnerabilities. Therefore we need to make a good shape or well-designed management process.

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RESEARCH ARTICLE

Gender Analysis of Farm Labours: A Case of Purulia District, West Bengal

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ABSTRACT

Gender equality and women empowerment is an important part of development. Women are the backbone of Indian Agriculture and their work has been still unrecognized worldwide. Women are one of the most important resources in agriculture. This paper is drawing an evidence of women's work participation in cultivation of Paddy and Mustard in a year. The analyze data shows that in the cultivation of paddy the women participate 54.4 percent of the workforce whereas the men comprise 45.5 percent of the workforce and their (women) total workforce is 1.2 times more than the men and in Mustard cultivation women participate 50.83 percent of the workforce whereas men engage 49.16 percent of the workforce. Calculating the total workforce in cultivation of Mustard it is seen that women's participation is 1.1 times more than the men. Apart from that ploughing step is predominantly men's activity which is more than women but in transplanting and weeding steps women are engaging much more than men which is quite a lot remarkable. Over all labor participation of rural women in agriculture and food production is exceeding the men's burden and is significantly increasing day to day. Women are making more contribution to agriculture and their diversity of work is observable but the work is still generalized and unrecognized. Hence, their (women) burden of work, time use in the committed work and the diversity of the work, keeping these in mind it is necessary to give them value for their labor/workforce.

Keywords: Women, Men, Paddy, Mustard, Agriculture workforce, Time use, Gendered nature.

INTRODUCTION

One of the most important principal of rural livelihood is agriculture and its allied activities. The word 'farmer' and the image which is coming to our mind immediately is that a man is working on farm land but the scenario is different now a day. Two villages (Tilabani, Taldi) of Purulia district are surrounded by tribal population. These tribal peoples' livelihood depends on mainly agriculture. Every household of those villages has their own land and they cultivate it by themselves, sometimes by hired labour. Both male and female share their labour in agricultural production. According to (2001) Census the total population of India is 102.87 crore, wherein, the male population is 53.22 crore and female population is 49.65 crore. Most of the women contribute their labour in household income through farm (landless agriculture labourers) as well as non-farm activities. Despite involvement in domestic work, the women contribute their labour force in farming related activities. Spending time in household work is not considered as valuable work and no credit is gone to the women household worker for those works. Traditionally, women do the exclusively tedious, time and labour intensive works like sowing, transplanting, weeding and intercultural operations, harvesting, threshing, transportation and post-harvest operations like shelling, cleaning, grading and processing etc. All these jobs involves considerable amount of drudgery, because it is mainly done manually (Shilparani, 2007). In most Indian families daughters are viewed as liabilities and on the other hand sons are considered as idolize and celebrity. In addition to the patriarchal culture, common in different degrees throughout the world, is the equally common problem that while women typically carry out most of the work inside as well as outside involved in caring for the home such work is given little or no social or economic importance, and as a result, women are perceived with little importance. While the work done by men is widely acknowledged and most men are considered as economically productive, women who are engaged in household work and farming work are classified as economically unproductive. Agriculture is the dominant occupation in rural areas and its activities are seasonal, many women join the labour force during the sowing and harvesting seasons and withdraw on the face of non-worth work (Acharya; Mathrani, 1992).

Damisa et.al (2007) highlighted in their study that despite of various social, economic and various other constraints women have high level participation in agriculture and they are very committed in their agricultural activity. Overall the level of involvement of women in farm decision making was found very medium. About 60 per cent of agricultural operations like sowing of seeds, transportation of sapling, winnowing, storage of grain etc. are handled exclusively by women, while in other jobs they share the work with men. Apart from participation in actual cultivation, women participate in various forms of processing and marketing of agricultural produce (Aggarwal, 2003). Within agriculture labour force, the proportion of women is more compared to men and their contribution in agriculture and farm activities is also greater (Arunkumar et al., 1994). Roy (1992) found that the incidence of women agricultural labourers is not only very high in Bihar, but there are wide variations among the different districts in this regard.

Although there is large divergence in the incidence of women labour even within the plains of Bihar, it is generally higher there than in the plateau region, which has substantial proportion of scheduled tribes. Hence, the present investigation aims at time utilization by women as well as by men in crop production during two certain seasons of a year. Singh and Vinay (2012) briefed in their working paper about the significance of female labour in agriculture and allied activities. They further stated that the role of women in agriculture as female labour is not highlighted in India. In spite of their presence in activities sowing, transplanting and post-harvest operations they are considered as an invisible workers. Women have played and continue to play a key role in the conservation of basic life supporting systems such as land, water, flora and fauna. They have protected the health of the soil through organic recycling and promoted crop security through the maintenance of varietal diversity and genetic resistance. Therefore, without the total intellectual and physical participation of women, it is not be possible to popularize alternative systems of land management to shifting cultivation, arrest gene and soil erosion, and promote the care of the soil and the health of economic plants and farm animals (Prasad & Singh, 1992). MunMun and Arindam highlighted the facts that women participation in agriculture is increasing with time and women are now acknowledged with the status of "agricultural worker". Though discrimination of wages and in working status still prevails for women labour but

due to implementation of various policies and initiatives taken by government the invisibility of women as an agricultural worker is plummeting and will further diminish in future (MunMun and Arindam, 2014). Hence, the present investigation aims at time utilization by women as well as by men in crop production during two certain seasons of a year.

Objectives

1. To identify the gendered nature in cultivation of Paddy and Mustard during Kharif and Rabi season.
2. To compute the time use with respect to the above male and female farm labour.

METHODOLOGY

The present research work has been carried out at two villages of Purulia district of West Bengal during 2017-2018. During this work 25 farmers (male & female) were interviewed to collect the primary data. The method which is used is the qualitative and quantitative method of data collection. For the sampling, purposive sampling was carried out, to reach the respondent to collect the data snow ball sampling was used for getting the more data. In quantitative method the selected population information is analysed through statistical method. The analysed information has been arranged in tabulated form and interprets qualitatively to get clear information about that study.

RESULT AND DISCUSSION

Research has been done with the engagement of male & female farmers with different steps of cultivation of two different crops in a year. Hence, the salient findings of the study have been presented and discussed hereunder through different tables and figures.

Table-1and Figure-1illustrated that in terms of transplanting; weeding women contribute more than men. It astonishes that in transplanting step women participation is 2 times more and in weeding step women participate approximately 11 times more than the men. Apart from that in ploughing step only men participating 3.5 times more than women. Focusing on overall step it is found that women contribution in paddy cultivation is more than men.

Table-2 elaborated that in ploughing step men are contributing 4 times more than women and in Fertilizer/pesticide application women contribution is approximately 2 times more than men but in terms of overall participation it is found that women participation is more than men. During analysis the data it is seen that a man worked for 1595 hours in a year in one hectare of land whereas a woman worked for 1789 hours in a year in one hectare of land for the cultivation for Paddy and Mustard. Apart from that, Men were found to be doing 47.14% of the work whereas Women were found to be doing 52.87% of the work in cultivation of Paddy and Mustard in that area. It is also found that in overall participation a woman works 1.13 times more than a man.

CONCLUSION

Rural women are the major contributors in agriculture. Her range of work varies from crop production to livestock rearing and home maker. In spite of doing hard work or spending more time in agriculture it is still considered that women are not economically productive. After analyzing the data it is found that overall participation and time spend in cultivation of Paddy and Mustard during agricultural season women's work participation is more than men and their work should be recognized and considered as economically productive work. Women do the time & labour intensive works like sowing, transplanting, weeding and intercultural operations, harvesting, threshing, transportation etc. All these jobs involves considerable amount of drudgery, because it is mainly done manually. Finally I would like to conclude that women are equal to men, even this study shows that women are not only the

same as men but also they (women) are more hard worker, more committed than men in terms of work, in terms of time spend in different types of work.

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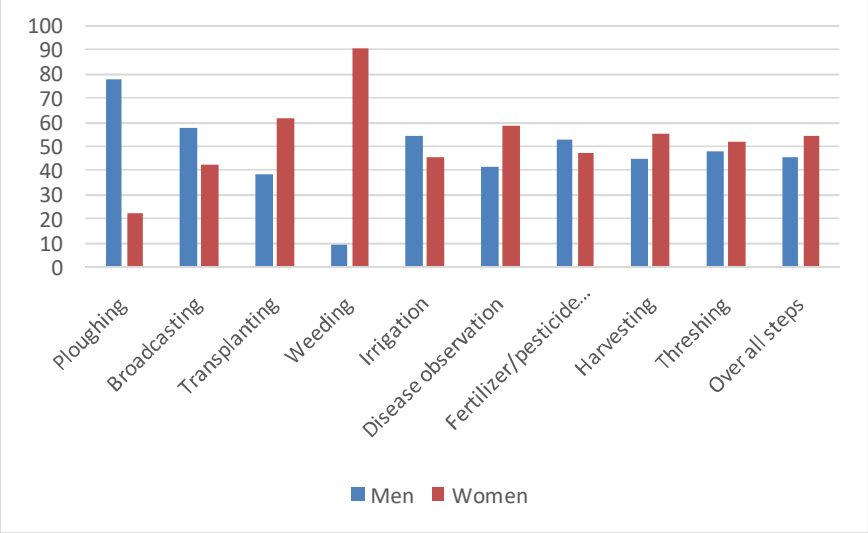

Fig.-1: Percentage of Labour step associated with Paddy production

Table 1: Percentage of Labour step associated with Paddy production

Labor Step(s)	Labor Steps in local language	Men (%)	Women (%)
Ploughing	Nahelsi	78.43	21.57
Broadcasting	Horoaafor	57.75	42.25
Transplanting	Hororoie	38.43	61.57
Weeding	Herhate	8.75	91.25
Irrigation	Siat	54.65	45.35
Disease Observation	Tijukomenakuase bang	41.30	58.70
Fertilizer/pesticide application	Turier	53.05	46.95
Harvesting	Horoirr	44.94	55.06
Threshing	Horodall	48.21	51.79
Over all		**45.5**	**54.4**

Table-2: Percentage of Labour step associated with Mustard production

Labor Step(s)	Labor steps in local language	Men (%)	Women (%)
Ploughing	Nahelsi	79.08	20.92
Broadcasting	Horoaafor	50.86	49.14
Earthing up	Kodaldhaka	53.17	46.83
Irrigation	Siat	52.88	47.12
Disease Observation	Tijukomenakuase bang	40.15	59.85
Fertilizer/pesticide application	Turie	34.58	65.42
Harvesting	Horoirr	45.12	54.88
Threshing	Horodall	45.08	54.92
Over all		**49.16**	**50.83**

Table 3: Percentage of Labour step associated with Mustard production

Labor Step(s)	Labor steps in local language	Men (%)	Women (%)
Ploughing	Nahelsi	79.08	20.92
Broadcasting	Horoaafor	50.86	49.14
Earthing up	Kodaldhaka	53.17	46.83
Irrigation	Siat	52.88	47.12
Disease Observation	Tijukomenakuase bang	40.15	59.85
Fertilizer/pesticide application	Turier	34.58	65.42
Harvesting	Horoirr	45.12	54.88
Threshing	Horodall	45.08	54.92
Over all		**49.16**	**50.83**

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RESEARCH ARTICLE

Collectivizing Community for Development Action: A Conceptual Framework

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ABSTRACT

The new way to deal with community development gives a change in perspective in the conventional methodology where the job of the administration is transformed from that of administration to assistance. It visualizes a base up approach whereby the dwellers' involvement themselves chooses their plan of action. Village improvement is a constant, pluralistic and broadly participatory procedure and fundamentally implies, progression of a territory, uncovering, unfurling or opening up something which is dormant and a change that is alluring. In spite of this, often people are not participating in developmental activities. Present article highlights the fact that Often to develop a good Development Plan one needs to do some activity which doesn't have any direct benefit to them, but have a great indirect benefit like the PRA activities. The challenges to collectivizing them are come from different angel like Women's participation, class, caste, religion, occupation of people, gender, political influence, literacy rate. These are all the problem came from the community itself. Some problem may also come from the team who is working there for development activities. Not only problems, but also the authors intend to ventilate some solutions. The faith on the team from the community side is very much important. If the team failed to build the relation or faith with the community then the Participation of the people will be nothing.

Keywords: Community Development, PRA, Village Development Plan, Participatory Planning

INTRODUCTION

Collectivizing community is the most difficult task to do any community program. The community participation depends on the work done with the community. The community based on different kind of people different mind-set of people. As per definition community is small or large Social Unit in a particular place which has something common like values, norms, religion, identity etc. But when we face the community in a village or any other place it seems to very diverse and mixed up different kinds of people are came together to form a community. The development action is the activities which people usually do with the people to develop them. Often the participation in development action is voluntary and need their important time.Thill (2011) led an investigation on model village and its supportable characteristic asset the executives, town self-administration, present day arrangements, participatory turn of events, movement, social value, bounty and genuine majority rule government of Ralegan Siddhi, situated in the drylands of Maharashtra. Anna Hazare, the famous social dissident has been the principle head behind the village development.Majumdar (2016) depicted in his study: It was discovered hard to credit to a specific plan/program the reasons of progress or disappointment in the formative procedure. Henceforth, in a workshop sorted out under the aegis of the Planning Commission in which the main NGOs and other rumoured establishments had additionally in a view was taken to embrace a territory based methodology for the assessment of the effect of the different plans of the Government of India. It is therefore the current examination has been done to record Angara square, Ranchi area, Jharkhand so as to consider Socio-monetary condition, populace and asset situation and to get ready collective intends to make a supportable model town. During the participatory exercise, the scientists understand the status of the locals during the whole course of movement on the grounds that the 'stick of control' was given over to them.

Problems to start a Community Action Plan

Often to develop a good Development Plan we need to do some activity which doesn't have any direct benefit to them, but have a great indirect benefit like the PRA activities. The challenges to collectivizing them are come from different angel like Women's participation, class, caste, religion, occupation of people, gender, political influence, literacy rate. These are all the problem came from the community itself. Some problem may also come from the team who is working there for development activities. The faith on the team from the community side is very much important. If the team failed to build the relation or faith with the community then the Participation of the people will be nothing.

Citing Example: Experience of a student of Azim Premji University

From our field experience the challenges we faced like, in our market visit we visited the place in the pick hour of their business, so the people were not willing to talk with us by keeping beside their business. So here time also play a big role to collectivizing people. In the whole market there were no women present. But we have women in our group, some of them was surprising to see the women there, some of them also didn't talk at all with the women. But when the women approaches to the people they didn't ignore they replied. But whenever they voluntary ask anything they ask them male person of the group. Many of them don't know about Azim Premji University and the course like Development. So the hesitate to answer, but in the same market we also find some people who know something about this type of project and field they helped us a lot. So here we can see the problem of reputation and knowledge works. When we visit the villages through FES, we saw a more people's participation there. It is just for only the reputation FES has there and the workers of FES earn the faith of the community of that area. In the beginning there was lot person they may thought that some new people came so we can get some new thing from them, but when we start doing our PRA the people start leaving the place. At last only few was left in that place to complete our work. That the case of productivity, whenever we have some productive for them they will be there for you, but this kind of thing which don't have any direct profit they doesn't show such interest to the activity. If we do any activity during their earning season we get least participation from the community.

The rural Poor people need money; they want those type of activity which will give the monetary benefit. So whenever we plan something we have to plan such a way that will help the people to income more directly or indirectly. In FES visit we see one point about language that language of the development action provider also has a great impact on the collectivizing process.

Everyone now agrees to the fact that increasing population and land fragmentation is going to affect human managed systems as well. Farming systems, in particular, is vulnerable to such changes. Since living has become more complex than before, human need, specifically food habits, has also been shifting rapidly and among the people consensus is on the move that alone farming cannot meet these growing demands of the people.

Proper communication, better grass root level penetration, cosmopolite source of information, regular involvement in different group and community activities had an important impact in enhancing livelihood, economic security and agricultural development. Without a good income it is difficult to sustain a livelihood, economic security could also not be maintained without proper income. If an individual is exposed to different activities and information sources in the society, he will be aware of certain things which will ultimately help in sustaining livelihood, maintaining economic security and agricultural development. Contact within the periphery is also an important factor.

Community Participation

Better mass media exposure, better interpersonal source and better interactive information are also an important factor in enhancing livelihood, economic security and agricultural development. Sufficiency in livelihood and economic security as well as agricultural development could be depicted through body language. Contingency communication, with its peripheral and cultural attributes also plays an important role in livelihood generation, economic security and agricultural development.

CONCLUSION

It is clear that institutions should vibrate the present condition of farm dwellers. It would create an impact on individual, family and community level. At individual level, institutions should help to raise yield, income and reliance of the family farms. At family level, institutions should ensure food security, sustainability and the role of women. According to peoples' perception, social inclusion and empowerment should be the ensured by the institutions.The problems here mentioned are the broad problem which a development practitioner has to face during his work. The problems have to know before hand before going into field to avoid problem faced during the activity. Need to know about the area and the people also reduce the challenges faced during collectivizing the community.

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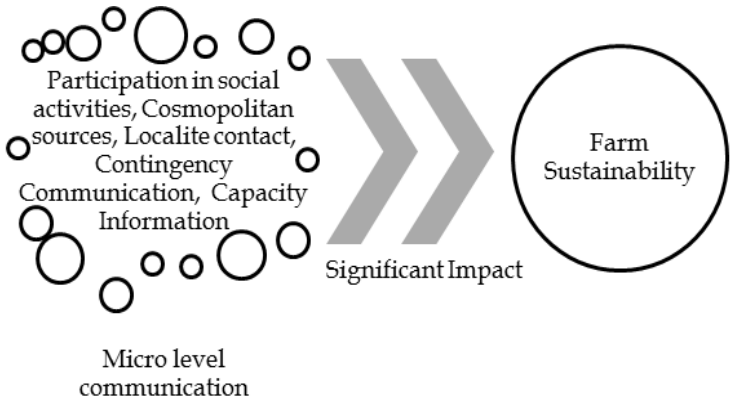

Figure 1: Participation and Community Impact

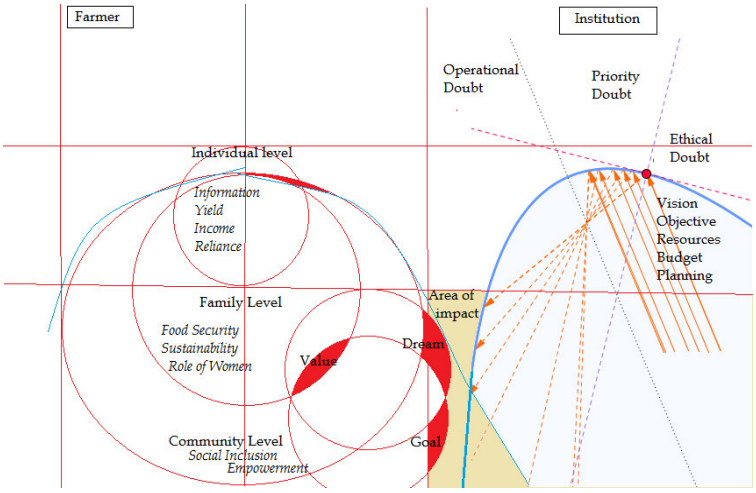

Figure 2: Policy Role and Community Participation

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RESEARCH ARTICLE

Sub Sector Analysis of Potato in Burwan Block of Murshidabad District

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ABSTRACT

Present study expects examine sub-sector analysis of 'Potato' in the Burwan Community Development Block in Murshidabad District. Production and Marketing are two Different things but are connected with a strong bond. Both are Complementary to each other. West Bengal is Second Highest Producer in the country but in every year lots of farmer getting fewer prices for their production, the issues like storage problem and export to other state are normal in every year. In West Bengal the marketing problem is more prevalent than the Production Problem. The main Market Problem is due to the middleman present in the chain. The farmers get very less amount due to this long chain of Middle Man known as *Forias*. The study is based on Quantitative and Qualitative both. Data Collection Methods was be based on Semi-Structure Interview and Focus Group Discussion. The Respondents were mainly Local Farmers, Traders and Market Operators. Snow-balling (will start the process from potato wholesaler) sampling method was applied for the Current Study. The Project was focusing to find the marketing channel of Potato in Burwan Block. This project may help the future work which will be done on marketing process or to find the problem in marketing. The work will give the proper idea of factors involving in marketing process and to find out the problem within the process. The project also help to focus on the role of Middle man in the marketing channel and help to eradicate the mal practice by the middle mans and wholesaler. The monopoly or duopoly can be successfully addressed through this study.

Keywords: Potato, Sub sector analysis, West Bengal, Middle man, Markeing linkage

INTRODUCTION

Potato belongs to the Solanaceae family, scientific name *Solanum tuberosum.* Among all the vegetables Potato is the most famous vegetable. Potato is the highest growing vegetable in India. The crop is used as a food crop as well with using as vegetable. The origin of Potato was in Andes in South America. According to FAOSTAT Data, 2018 India is the Second largest Potato producing Country in World. The Potato is very much reach with starch. The Nutrient content of Potato per 100 gms is,

1. Water	74.70
2. Carbohydrates (Starch and Sugar)	22.60
3. Proteins	1.60
4. Fiber	0.40
5. Fat	0.10
6. Minerals	0.60

Source

Potato in India, Central Potato Research Institute (CPRI), Shimla. In India Uttar Pradesh, West Bengal and West Bengal are the leading states on Potato growing. In India we use Potato with almost all type of Vegetables. Samosha, Masala Dosha, Alu Pratha are the most famous recipe of Potato. Potato is a mainly Rabi Crop, but now this days Kharif Potato also start cultivating. Potato sowing use to start in November-December and harvesting done in February-March. This is a subsidiary Crop. Except the northern districts of West Bengal in all districts Potato is cultivated. Hoogly, West Midnapore, Murshidabad are the leading districts in Potato production.

The Farmer sells the potato to the local middleman known as *Phorias* in West Bengal. Sometime the local cold storage owner also buys the whole potato from any farmer and act as a middle man. The Marketing process id followed by the chain of certain middleman to reach the ultimate consumer and most amount stored in the cold storage for future selling. The Storage was also done by the middle man. The middle man buy the product from the just after harvest.
There are a lot of problem is present in our current marketing System. This current study will focus on prevail Sub Sector in the study are and try to find out the problem within the Sub Sector. The price of the Market is very much fluctuating according to the marketing channel and the season. But the main profit use to go to the middle man, the producer didn.t gets any profit due to high price in retail market.

Main Objectives

To understand and conduct sub-sector analysis of 'Potato' in the Burwan Community Development Block in Murshidabad District.

LITERATURE REVIEW

There are different constrains of Potato Marketing in West Bengal. High marketing cost and margins, wide price fluctuations, existence of large number of middlemen, storage and transportation bottlenecks and lack of other marketing infrastructures are some constrains listed. They noted Potato Market as an oligopolistic in nature where commission agents dominate (Pandit et. al, 2003).
Price fluctuation is a common phenomenon in case of seasonal and perishable commodities like potato (Sharma and Sharma, 1996; Malik et al., 1995).

The price fluctuations are very important component for both for producers as well as for consumers. The growers have to sell off their produce as quickly as possible after harvesting because of perishable product and the oncoming hot summers. It is not possible for them to take the advantage of high prices during the off-season. Traders and big

farmers earned more profits by storing the potatoes and sell them in off-season moths. On the other hand price fluctuations in retail level effect the ultimate consumer (Arya, 1995).

Some of the conditions for effective potato export are economic feasibility, comparative economic advantage, quality standards, availability of export surplus, development of infrastructure relating to transport, storage and processing, organizational arrangement for export and export-import policy. For tapping the foreign markets we have to be more quality conscious, should have a state-of-the-art market infrastructure and long term export strategy (Dahiya and Bhati, 1992)

Potato has to go through a number of intermediate markets to travel from the producer to the consumer. But apart from the wholesale markets at various stages and the final retail market, there is an active bond market for potato (Mitra and Sarkar, 2003). Indian farmers typically depend heavily on middlemen particularly in fruits and vegetable marketing. The producers and the consumers often get a poor deal and the middlemen control the market, but do not add much value. There is also massive wastage, deterioration in quality as well as frequent mismatch between demand and supply both spatially and over time (Subbanarasiah 1991, Singh M et.al. 1985).

The Producer --Wholesaler – cum – Commission agent - Retailer - Consumer is the major marketing channel for Potato. More than 60% of total production marketed through this channel. The major constraints for Potato growers are higher production expenditure, higher price fluctuation, lack of marketing information and lack of transportation facilities. To overcome these problems, the provision of cold storage facilities to the farmers at village level, adequate transport facilities for the export of Potatoes, availability of market information to the farmers, establishment of vegetable co-operative marketing societies and fixation of minimum/maximum prices of potato as well as other vegetables are some of the means suggested to improve the efficiency of marketing of potato in the state (Jadav et. al., 2011).

Study Design

The study is based on Quantitative and Qualitative both. Data Collection Methods was be based on Semi-Structure Interview and Focus Group Discussion. The Respondents were mainly Local Farmers, Traders and Market Operators. Snow-balling (will start the process from potato wholesaler) sampling method was applied for the Current Study.

Selection of Study Area

West Bengal is selected purposively as West Bengal is the second Highest Potato Producer in Our Country according to Monthly Report, May 2018 by Horticulture Statistic Division. Among all the districts in West Bengal, Murshidabad is a leading Vegetable grower in West Bengal. The Block Burwan is selected as it is the Second Highest Potato Producer in Murshidabad District according to District Statistical Handbook 2014, Murshidabad. Also, the study area is selected to avoid Language barrier.

RESULT AND DISCUSSION

The project work was done in the Burwan Block of Murshidabad District in the time period from November to December 2018. The project was targeted to find the Sub Sector of Potato within the Burwan Community Development Block. The study was done through Snowball sampling method in three layer i.e. Wholesaler, Farmer and Retailer. Total No of Respondent was Wholesaler 11, Retailer 17 and 23 farmers. The above mention chart is an overview of the Sub Sector in this Block. The Burwan Block Potato market is Potato market in the Murshidabad District. The Burwan block is west most part of Murshidabad District. The area is very well known for its farming activities, especially for Potato. This area falls under the Mayurakshi river basin, which is known for good quality alluvial soil and the floods happen almost every year, helps the field to enrich themselves. The Burwan block has its four main village, those are Burwan itself, Dakbangla, Panchthupi and Kuli. Dakbangla is no itself a village, the

village name is Gram Salika. The Burwan block has very good road connectivity with other part of West Bengal. Badsahi Road connecting Durgapur express way and NH34 went through the middle of this block. Nearest railway stations are Rampurhat, Sainthia and Salar. The whole trade is done through the Dakbangla Market. Sunil Ghosh and Sushil Jain are the two main Potato seed traders in this market.

The Seed Potato Sub Sector is a part of the Main Sub Sector. I represent it separately to get a better understanding. The region is mainly cultivated the Hybrid variety of Potato i.e. 'Pokhraj'. The other varieties; like Jyoti, Chandramukhi also cultivated but in a very less area. The Hybrid Seed mainly imported from Punjab. There is a monopoly of seed farm, who supply seed potato to the wholesaler in Dakbangla. There are only two wholesalers in Dakbangla who import the seed directly from Punjab. But there are at least 10 to 15 wholesalers who use to sale Potato Seed in Dakbangla and Burwan. The farmers have a good social relationship with any or some of the Wholesaler and they used to buy seed from that wholesaler only. The price of the seed potato is decided on the basis of the current rate of Potato. The price of seed potato used to stay low than the current price of market. If the price of seed potato goes high then the old potato which was stored came into the market as seed potato. The yield rate of this two has some variation, so they choose the new F1 hybrid Variety generally yet there is no such price deference. As an adjacent block to the other district the wholesaler also sell the seed Potato to the nearby districts. The sold the Seed Potato to the local farmers in a slight higher rate. The price of seed potato varies from 200 to 350 rs/50kg Bag depend upon the weather condition and market condition. Transportation authority helps a lot to bring the Seed Potato from Punjab to Burwan. That is an integral part of this Sub Sector chain also.

The potato market is fully depending on the weather and market of adjacent state. The market is totally controlled by Public no government authority either APMC or Food Commission doesn't play any role. The storage activity has a great role in this marketing process also. Government has a role to fix the opening and closing date of cold storages and the rate of Cold storages. There is no auction process happen for Potato. Farmers sellthe product to any wholesaler where he can find better price and can store the potato by their own. If we divide the farmers into two part i.e. small and big then we can again find two different technique of selling Potato. Big farmer sale their product directly to the wholesaler or store it into the cold storage by their own by making a 'Bond'. Function of the Bond I will discuss later. The big farmer sometime has a good social relation with the wholesaler so they usually sell the product to them only. In every village there are a group of people who are the farmers or sometime not the farmers; they play the role of middle man in the villages. There are some fixed people who known in the villages as a middle man and that is their occupation. But there is no fixed middle man there; any people can emerge as a middle man at this time. Who collect some Potato from the local small farmers and take them all to the wholesaler in Dakbangla and Burwan town.

The local middle men are known as 'Forias'. The selling of Potato is not there main occupation, some of them have shops, some of them are farmer who do this activity in every season. The Forias all time not sell the full product to wholesaler, some time they also store the product in cold storage for better price. Mainly the small farmers sell their product to the Forias for immediate cash and not taking the responsibility of transporting the product to the wholesaler. The numbers of Forias aredepending on how much the production happens and other factor. There is fixed no of Forias like the wholesaler. From wholesaler side they give two option to the farmers, one the farmer should come with their potato to their shop and sell it to them and sometime the wholesaler come to the field and check the quality of potato and buy it from the field and take it to his shop by his own transportation. In this two case there are some slight price differences happen. The price obviously depends on the quality of potato, size of potato not on the amount produce. The Sub Sector has different stage to reach the consumer and in every stage the price of Potato get revised. The Price has increased in a large extend when the potato stored in to the cold storage and then marketed. The pricing of the potato is fully depending upon the market outside. Like Uttar Pradesh market. Uttar Pradesh is the highest Potato producing state in the country and West Bengal is Second. So the pricing in west Bengalis very much depend on the UP Potato market. The big wholesaler also export the potato to the neighbouring state depend on the price. The local market price is depending on the Bankura Potato market price.

When someone stores the potato in the cold storage they make a Bond of that potato. In the Bond it is written like the amount of Potato stored and the price of potato when it is stored. The owner can sell the bond to any one and then the other person will be owner of this potato. The big farmer sometime does this technique to get more prices. In Cold storage we need a huge amount of labour. Storing of Potato and when it comes out it needs a dry period by spreading in a place and again to pack it. This whole process need some labour, all the cold storage provide the labour by charging the money from the Potato owner. In Burwan Block there are two cold Storages. They follow the government prescribed charge for storing Potato. It varies from 70 to 80 rupees per bag. The rate is same if anyone store it for 3months or 9months. The transporter also have a huge role in this whole process like take the potato from field, taking it to store, from store to market. In every stage it needs the transporter. The some wholesaler has their own transport and some have to rent the transport.

The selling price of Potato starts from 100-200 rs/50 kg Bag from the field and reach up to 250-1000 rs/50 kg Bag in Local market. The whole price increasing is due to different stage of Sub Sector and the storing cost.

CONCLUSION

The Project was focusing to find the marketing channel of Potato in Burwan Block. This project may help the future work which will be done on marketing process or to find the problem in marketing. The work will give the proper idea of factors involving in marketing process and to find out the problem within the process. The project also help to focus on the role of Middle man in the marketing channel and help to eradicate the mal practice by the middle mans and wholesaler. The monopoly or duopoly can be successfully addressed through this study.

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RESEARCH ARTICLE

Challenges in Self-Employed Livelihood Strategies: A Study of Clay-Doll Makers Around Krishnanagar in Nadia, West Bengal

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ABSTRACT

Artisans who indulge themselves in this source of livelihood cast clay dough into making varied types of products. Potter communities transform clay dough into vessels and utensils, while there is another group of artisans who make mythological idols. There is another group of artisans who are observed to make small dolls, toys, sculptures, miniatures of mythological idols etc.However, not much focus has been given by researchers in this field as this a slowly dying field. This study was carried out in purposively selected hamlets of clay doll makers in Krishnanagar, Nadia district of West Bengal. Both primary and secondary sources of data were used for completing this study. Finally, the study reveals some technological aspects of doll making industry. There have been some technological innovations in the process of clay doll making over the years. A soil mixing machine is used to bring in the right consistency of clay. However, the artisans do not make much use of this machine since they prefer hand mixing of clay. Casting machines are used by artisans to cast bronze dolls and figurines. Gas burners are used to dry the clay figurines when there is deficit of sunlight during the monsoons. It is also used be artisans to speed up the process of doll making.

Keywords: Clay dolls, Krishnanagar, Mythological idols, Soil mixing machine, Potter communities.

INTRODUCTION

The initiation of clay doll making emerged in West Bengal during the era of British Rule when Raja Krishna Chandra Roy of Krishnanagar, Nadia District developed an interest in art and music. He brought in communities of various artisans and craftsmen from Dhaka and surrounding areas which included potters, clay doll makers, idol makers, musicians, etc. have resided in various hamlets of the district for generations now. Earlier, they used to reside in

different hamlets according to the castes that they belonged to but presently, however, intermingling of the caste groups have taken place thus bridging the gap between the groups.

Clay doll making has been a prominent source of livelihood for several communities from different districts of West Bengal such as Purulia, West Midnapore, Burdwan, Birbhum, Murshidabad, Nadia and Kolkata. Kumortoli in Kolkata and Krishnanagar of Nadia have gained popularity for mastering proficiency in idol making and clay doll making respectively. Exhibitions of clay dolls of Krishnanagar are hosted in several countries.Paul (2017) in his article discusses about the fact that with the emergence of an alternative market dolls i.e., dolls made of plastic and fibre dolls, have decreased the demand for clay dolls. The cost of production and the time taken in producing each units of dolls in this new sector is much lesser than the traditional dolls thereby widening the gap between the market value of both types. He further argues that the work done behind making clay doll is extremely laborious and exhausting. Also, the occupation is seasonal in nature as the clay gets dried up very easily in the summers causing it to break; thus there is a tendency among the artisans to switch to an alternative source of livelihoods like construction work. In some parts of West Bengal, it has been observed that some communities of artisan migrate in search for better standards of living or they migrate to places where there is a higher demand for the skill.

The artisans also work in very compromising conditions with poor infrastructure with middlemen often exploiting the artisans by not paying their dues. Clay doll making reflects the thought process and perception of the artisans and often represents the stories of certain caste, class or community of the society or reflects the myths and beliefs of a region. Majumdar (2016) talks about the livelihood of wooden doll makers and how their monopoly in the market is lessened by the day because of the emerging love for Chinese products among the public. The government and the handloom industries helped in shaping the journey of doll making was established but owing to factors like rapid urbanisation, advancement of technology and the interference of the Chinese market has led to the artisan's product and this heritage art of Bengal towards destruction. Through a gendered perspective, men are observed to dominate the carving of the the teak wood and make a shape of the doll while the female population engages themselves with the painting of the products. He mentions that as an alternative livelihood, doll makers often involve themselves in their ancestral lands but however, some families solely depend on doll making. They reach out to the market either individually or they form a cluster of artisans and the mass produce from the cluster is sold to the consumer. Jana (2015) in his study on the community of the clay-doll makers of Nadia, West Bengal talks about the factors leading to product development which financial assistance to improve the quality of the product, marketing and the communication with the consumers, proper infrastructural facilities such as packaging and storage, weather conditions suitable for doll making, etc. In his study with the respondents he understood the need of the artisans to be up-to-date with technological innovations, consumer demands, etc. so that can manufacture products without incurring major losses.

Hazra (1991) discusses how the needs and demands of the higher classes do not match with the traditional heritage and culture of art in West Bengal. He also mentions Similar to the other authors, it has been also mentions about the commercialisation of plastic puppets, soft toys and modern dolls through Chinese dumping has led the potter and artisan communities of Bengal in a vulnerable condition. Apart from this, factors like the government's efforts in safeguarding the art has lessened considerably, rapid urbanisation and modernisation in individual consumer's choices has led to the drastic decrease in the demand for clay dolls. Hazra (2017) in his article explores the fact that the unavailability of a proper market with enthusiastic consumers who feel passionate about the craft has influenced the decline of this art and cultural heritage of Bengal.

Objectives of the study

- To study the challenges faced by clay doll makers.
- To understand the livelihood diversification adopted by the artisans.
- To study how gender plays a role in the clay-doll making process.
- To understand how technological innovations in the doll-making process have impacted the lives of the artisans

METHODOLOGY

The research was a qualitative study which was conducted through in-depth semi-structured interviews with the respondents. I have had interactions with 15 independent artisans and 5 contractual labourers in a hamlet named Ghurni in Krishnanagar. However, since the population of the hamlet have been associated with same source of livelihood for decades now, the responses of the respondents have been similar. The residents of the hamlet face similar issues with their livelihood that is connected to clay doll making.

FINDINGS

Age

Most commonly it was observed that the artisans who associated themselves with the craft were essentially mid aged. The younger generation rarely associated themselves with the craft since they engaged themselves with salaried jobs. The scope for career growth has become very limited over the years owing to the decline of the culture of clay doll making. Of all the artisans I have interacted with, 9 artisans were from the age group of 31-50. There were 8 artisans who were aged more than 50. There were only 3 artisans who were aged less than 30. Supriyo Pal, 28 after completing his graduation had got into the business of clay doll making. He said, "I had to take up the family business after my father's sudden death so that I can support my family financially".

Education

Owing to critical financial situations in households and travelling long distances to access education it was observed that two out of the nine artisans from the older generation were illiterate and have had no formal education. However, three artisans have been able to complete their graduation from the same age group. Others have had to leave their education in between in order to financially support their families. A common pattern observed among the mid-aged artisans was that they have just been able to complete their education up to standard ten. This generation although envisaged themselves to be further educated and pursue different careers but were unable to do so due to familial responsibilities. Among the 3 young generation artisans, only one was able to finish his graduation while the other two had just been able to complete their primary education. The younger generations of artisan families in Ghurni hamlet have access to good schooling with advanced infrastructure and comparatively lower fees which are why they are mostly graduates. However, none except one artisan had any formal education on the craft of clay doll making. All artisans have mastered the skill from their early childhood through the help of their forefathers. The exceptional case of Gautam Paul is noteworthy since he coalesced the traditional craft of clay doll making with contemporary art forms through his formal education in Accademia di Belle Ardi di Brera, Milano in Italy.

Caste

Earlier when clay doll making was in its emerging stage, only the Pal community (who belonged to a higher caste) were the ones who associated themselves with the craft. However, with generations of artisans making use of this craft as a source of livelihood, a lot of intermingling have taken place. People belonging to other communities such as Mullick, Bagdi communities, etc. who are from lower castes now connect with the craft. People who are indirectly involved in clay doll making process: Other than the stakeholders which include the artisans and the entrepreneurs who run their own studios, and consumers, there are other people who are connected with the process of doll making. Rickshaw pullers are responsible for transporting soil from the fields to the studio of each artisans for which he receives Rs. 200-300 for each trip that he covers. Soil mixing labourers are accountable to remove unwanted objects from the soils and making clay doughs of the right consistency. They get a remuneration based on the amount of soil that needs to be segregated and mixed which ranges from Rs. 100-300. Painters give the finishing touch to the clay moulded dolls and other products. They are also compensated on a contractual basis where they have to paint an average of 450-500 dolls for which they receive Rs. 800-1000. Middlemen also play a role in the

process of clay doll making where they connect the artisans to the wholesalers and consumers. They make individual profits in the business.

Changes in the process of clay doll making

Technological innovations: There has been some technological innovations in the process of clay doll making over the years. A soil mixing machine is used to bring in the right consistency of clay. However, the artisans do not make much use of this machine since they prefer hand mixing of clay. Casting machines are used by artisans to cast bronze dolls and figurines. Gas burners are used to dry the clay figurines when there is deficit of sunlight during the monsoons. It is also used be artisans to speed up the process of doll making.

Quality of paints

Earlier, natural colours were used to paint the dolls but they did not have a long lasting effect and the colour would very easily faded. Also, there weren't a lot of options to choose among the natural colours. With the evolution of acrylic and synthetic paints and primers, there has been significant improvement in the quality of the clay dolls that were produced. The dolls were obviously more attractive because of a glossy texture and a varied number of options to choose from. Primers help in making the colouring more durable.

Use of mould

The artisans make their own moulds out of Plaster of Paris in cases of bulk orders. This helps the artisans in making the exact same product and also speeds up the process of doll making.

Social media and digital marketing

Social media has helped the artisans to advertise their products much more efficiently which eventually helps in better sale of their products. They also have easy access to contemporary and new designs through the internet.

Use of alternative raw materials

Sometimes when the correct consistency of clay is not achieved, it becomes very difficult to mould the dolls and they often develop cracks. So to overcome this challenge, the artisans have succumbed to other alternative raw materials like fibre, marble, stone dust and bronze. The cost of production in case of fibre and stone dust is much lower than that of clay while in case of marble and bronze the durability id much higher.

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RESEARCH ARTICLE

In silico Analysis of the Long Pepper as Targeted Therapy for Targeted Disease Tomato Yellow Leaf Curl

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ABSTRACT

As local wellsprings of medications, remedial plants are used from the out of date events. Long pepper is one of the significantly used potential restorative plants on the planet. This plant is usually used for the treatment of standard chilly, free insides, fever as a result of a couple of infective explanation, jaundice, as a prosperity tonic for the liver and cardiovascular prosperity, and as a malignancy anticipation operator. It is furthermore used to improve sexual dysfunctions and fill in as a prophylactic. All bits of this plant are used to isolate the dynamic phytochemicals, yet the structures of phyto constituents by and large fluctuate beginning with one area then onto the following and with spot, season, and time of gather. We are using this property of Long pepper to get some new meds for Yellow Leaf Curl. The jobs of various pesticides, added substances, etc change the sustenances into poison. Other than the responses of these pesticides and added substances, etc are hazardous as considering the way that it prompts initiation of different dangerous development. In this whole world, the amount of patients passing on from threatening development is extending in a bargaining way. In-silico examination has done using programming and we further centered around a part of the characteristics at risk for Yellow Leaf Curl and pharmacophores from Long pepper and decimated some silico assessment. In this we have found that these two pharmacophores are having better Mol Doc score from any others. From this we can find that these two pharmacophores can be a response for pesticides in not all that removed future.

Keywords: Yellow Leaf Curl, Docking, *In Silico* Analysis, Pharmacophore, Long pepper.

INTRODUCTION

Long pepper was furthermore a generally adored in spiced wines and digestives. Half-fix, half-inebriant, spiced alcoholic cordials have been around since the Romans, the most renowned and enduring of which seems to have been the medieval 'hippocras', a red or white wine, instilled with mix of flavors and improved with sugar or nectar. In any case, in spite of the way that the Greek pro Hippocrates was various things, he was not the fashioner of vinum hippocraticum. Or on the other hand possibly, the authentic foundation of this particular beverage was gotten from the condition of the tightened channel through which the spiced wine was focused on, alluded to vintners as a manicum Hippocraticum – Hippocrates' sleeve. In spite of the way that creation procedures changed all through the many years, the name, and man's fulfillment in it, stuck, and references to hippocras can be found well into the eighteenth century.

Piperine has been seemed to overhaul the bio-availability of fundamentally and remedially contrasting medications, maybe by adjusting film components, as a result of its straightforward distributing extending vulnerability. The effect of Trikatu', a compound Ayurvedic availability containing Piper longum as one of the huge fixings, was attempted in mix with various meds. The examination uncovered that Trikatu' extended their profile availability either by propelling speedy digestion from the gastrointestinal tract or by protecting the medicine from being used during its first section through the liver in the wake of being expended, or by mix of the two instruments.

Studies have been done to affirm the ordinary instances of Ayurveda for antiasthmatic development of Piper longum. A concentrate of the natural items in milk decreased idle cutaneous excessive touchiness in rodents and made sure about guinea pigs against antigen-started bronchospasm. Piperine was evaluated and found to apply significant protection from tertiary butyl hydroperoxide and carbon tetrachlorideinduced hepatotoxicity, by diminishing both in vitro and in vivo lipid peroxidation. A characteristic item remove was reviewed in rodents for its hepatoprotective action against CCL,induced exceptional, incessant and reversible mischief and steady irreversible damage, using morphological, biochemical and histopathological assessment parameters. The concentrate improves the recuperation technique by keeping fibrosis, yet offered no protection from exceptional mischief or against cirrhotic changes.

Bound piperine exhibited a central energizer action in frogs, mice, rodents and dogs and extended the rest actuating response in mice. It irritated respiratory trouble impelled by morphine or pentobarbitone in anesthetized dogs and an oil ether concentrate of the normal items distanced morphine-instigated respiratory sorrow in mice, A comparative report coordinated with piperine and nalorphine, for impacts against morphine-provoked respiratory demoralization and absense of agony, found that both exchanged respiratory hopelessness regardless, rather than nalorphine, piperine didn't compromise morphine-activated absense of torment in rodents.

MATERIAL AND METHODS

Phytochemicals of Long pepper have been listed with their structure data files which are taken from pubchem ChEBI. Genes has been taken randomly for Yellow Leaf Curl using NCBI database. Table 1 has been showing the enlisted pharmacophores and the targeted genes. The PDB numbers of gene are taken from RCSB. The In-silico analysis has been done using BIOVIA –Discovery studio. We have performed various docking and used the Ramachandran plot and others.

Protein identification and preparation

The announced atomic targets liable for Yellow Leaf Curl are taken (Table 1) and the X-beam crystallographic structures of these objective proteins were recovered from protein information bank (PDB). The recovered PDB structures contain water particles, substantial iotas, cofactors, metal particles and so forth and these structures don't have data about topologies, bond requests and formal nuclear charges. Thus the downloaded PDB structures were readied utilizing 'plan protein' convention of Discovery Studio 4.0. The objective proteins were set up by evacuating

all water particles, ligands and other hetero molecules from the structures. Hydrogen iotas were added to the particles to fulfill their valencies. The structures were then vitality limited by applying CHARM power field to evacuate the steric conflicts between the molecules so as to get steady adaptation.

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The binding sites of the receptor proteins were predicted based on 'receptor cavity method' using Accelry's Discovery Studio 4.0. Using this protocol, active sites of the target receptor were identified based upon the inhibitory property of the amino acid residues present in the binding sites.

Ligand preparation and filtration

An arrangement of 4 phyto mixes from Long pepper was taken as ligands for docking assessment. The 3D structures of these mixes were downloaded from PubChem database. These ligands were then tidied up, chose 3D supports and made ligand modifications by applying 'plan ligand appear' of Discovery Studio 4.0. After readiness, the mixes were disconnected dependent on the atomic properties for anticipating their dissolvability and helplessness in quiet exposure. The most standard of the physical property channels is Lipinski's "rule-offive", which spins around bioavailability. The standard conveys that the mixes have atomic mass under 500 daltons, not in excess of 5 hydrogen security advocates, not in excess of 10 hydrogen security acceptors and an octanol-water area coefficient log P not more obvious than 5 (Lipinski et al.,2001). The separated mixes were then utilized for docking evaluation.

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The antimicrobial activity of all the 4 phytochemicals definite from Long pepper was assessed by docking these blends against the specific powerful districts of the goal proteins. Divulgence studio 4.0 was used in this assessment to find the teaming up blends of Long pepper with the picked focal points of Yellow Leaf Curl . Strategies of Discovery Studio 4.0 are to completely dock or score potential spots of each ligand in the coupling site of the proteins. Docking examination of the target proteins was done with regular blends got from Long pepper to find the supported course and limiting attachment to the blends in with each target protein using scoring limits. A sub-nuclear components (MD) imitated toughening based computation, explicitly, CDOCKER was used to score the partner blends. This methodology uses a gridbased depiction of the protein-ligand potential associations with figure the coupling affection (Wu et al., 2003). CDOCKER uses sensitive focus prospects, which are viewed as fruitful in the age of a couple of unpredictable adjustments of little organics and macromolecules inside the dynamic site of the goal protein. Ligands were docked to the proteins followed by scoring them for their general nature of collaboration to recognize opportunities for sedate progression. The last positions were then scored subject to the supreme docking imperativeness, which is made out of intramolecular essentialness of ligand and the ligand-protein affiliation. The most negligible essentialness structure was taken as the best fit. Comprehension of the characteristics was done using measures gave by Discovery Studio, for instance, CDOCKER imperativeness, CDOCKER joint effort essentialness, hydrogen bonds, confining imperativeness, etc.

Drug likeliness

Medication resemblance is a subjective idea utilized in sedate structure to assess how the substance demonstrations like medication regarding factors like bioavailability. The atomic properties which impact assimilation, conveyance, digestion, discharge and harmfulness are perceived as a long side remedial intensity as key determinants of whether a particle can be effectively evolved as a medication (Zhang et al., 2012). These parameters are answerable for around 60 percent disappointments of all medications in the clinical stages thus the expectation of ADMET properties assumes a noteworthy job in new medication disclosure process (Hire et al., 2012). In this manner, it has gotten basic to configuration lead mixes which would be effectively Breast ly ingested, handily moved to their focused on hand of activity, not effortlessly changed over into poisonous metabolic items and effortlessly dispensed with from the body before amassing in adequate sums. The ADMET properties of the mixes were investigated for medicate like up-and-comers.

RESULT AND DISCUSSION

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The three dimensional structures of the identified target proteins were retrieved from the protein data bank. PDB ID of the targeted protein structure are mentioned in Table 1.

Ramachandran Plot of the targeted gene

The Ramachandran plot is among the most focal ideas in auxiliary science, found in distributions and course readings the same. Be that as it may, with the expanding quantities of known proteinstructures and more noteworthy precision of ultra-high goals protein structures, we are as yet getting familiar with the essential standards of protein structure. The utilization of torsion edges to portray polypeptide and protein adaptation was created by Sasisekharan as a major aspect of his investigations of the structure of collagen chains during his work as an alumni understudy in the exploration gathering of G.N. Ramachandran. The intensity of this methodology was promptly clear and its utilization immediately got broad. Utilizing updated definitions, this alleged Ramachandran plot or φ, ψ-plot has remained almost unaltered in the resulting fifty years and keeps on being a necessary instrument for protein structure research and instruction.

Hydrophobicity Plot of the Genes

Protein–protein interactions (protein functionalities) are mediated by water, which compacts individual proteins and promotes close and temporarily stable large-area protein–protein interfaces. In their classic article, Kyte and Doolittle (KD) concluded that the "simplicity and graphic nature of hydrophobicity scales make them very useful tools for the evaluation of protein structures." In practice, however, attempts to develop hydrophobicity scales (for example, compatible with classical force fields (CFF) in calculating the energetics of protein folding) have encountered many difficulties.

Ligand preparation

4 of the pharmacophores are fulfilled Lipinski rule and are relied upon to be dynamic mixes after Breast organization. The ligand particles with least restricting vitality are considered as mixes with most noteworthy restricting liking. This coupling proclivity showed an engaged collaboration between the above mixes with the objectives contrasted with others. The parameters for finding the best inhibitors, for example, CDOCKER vitality, CDOCKER cooperation vitality and number of hydrogen bonds were additionally assessed. CDOCKER vitality is the joined vitality delivered by the entirety of inward ligand strain vitality and receptor-ligand collaboration vitality where, CDOCKER cooperation vitality is the association vitality between the protein and ligand and the estimations of these two parameters show the quality of communication between the proteins and the ligands. Other than least restricting vitality, mixes with least nuclear vitality distinction between CDOCKER vitality and CDOCKER collaboration vitality were dissected. In view of CDOCKER vitality and CDOCKER collaboration vitality, Fig 4 is indicating the outcome ADMET Analysis:

Considering the comparable CDOCKER energy, interaction energy and binding energy, three compounds were forwarded for ADMET analysis. These studies are based on the ADMET(Absorption, Distribution, Metabolism, Excretion and Toxicity) properties of the compounds. These properties provide insights in to the pharmacokinetic properties of the compounds and were checked using Discovery Studio's built in ADMET protocol. The various parameters tested in this study were aqueous solubility, Blood Brain Barrier (BBB) level, Hepatotoxicity, Absorption level, AlogP and CYPD26. Pharmacokinetic properties of the best fit phytochemicals showed that two of the compounds had passed all the pharamacokinetic parameters. The compounds that passed the parameters were N-methyltyramine and dalbergioidin. These compounds were thus selected as the best compounds in this study as they had good interaction scores along with ADMET properties.

CONCLUSION

The apparent pharmacophores can be bound from the Long pepper and can be progressed as the ordinary solution for the Yellow Leaf Curl which is having lesser awful sign from the chemotherapeutic medication open in the market. This medication will in like way be incredibly progressively reasonable from the accessible drugs and these prescriptions are additionally not ruinous for the average cells as they are gotten from the common things.

The stand-apart fragment of the assessment is to focused quality treatment for biopesticides. This will assist our future medication with being totally identified with the Pharmachophores and the organizations of created and threatening development causing medication will reduce.

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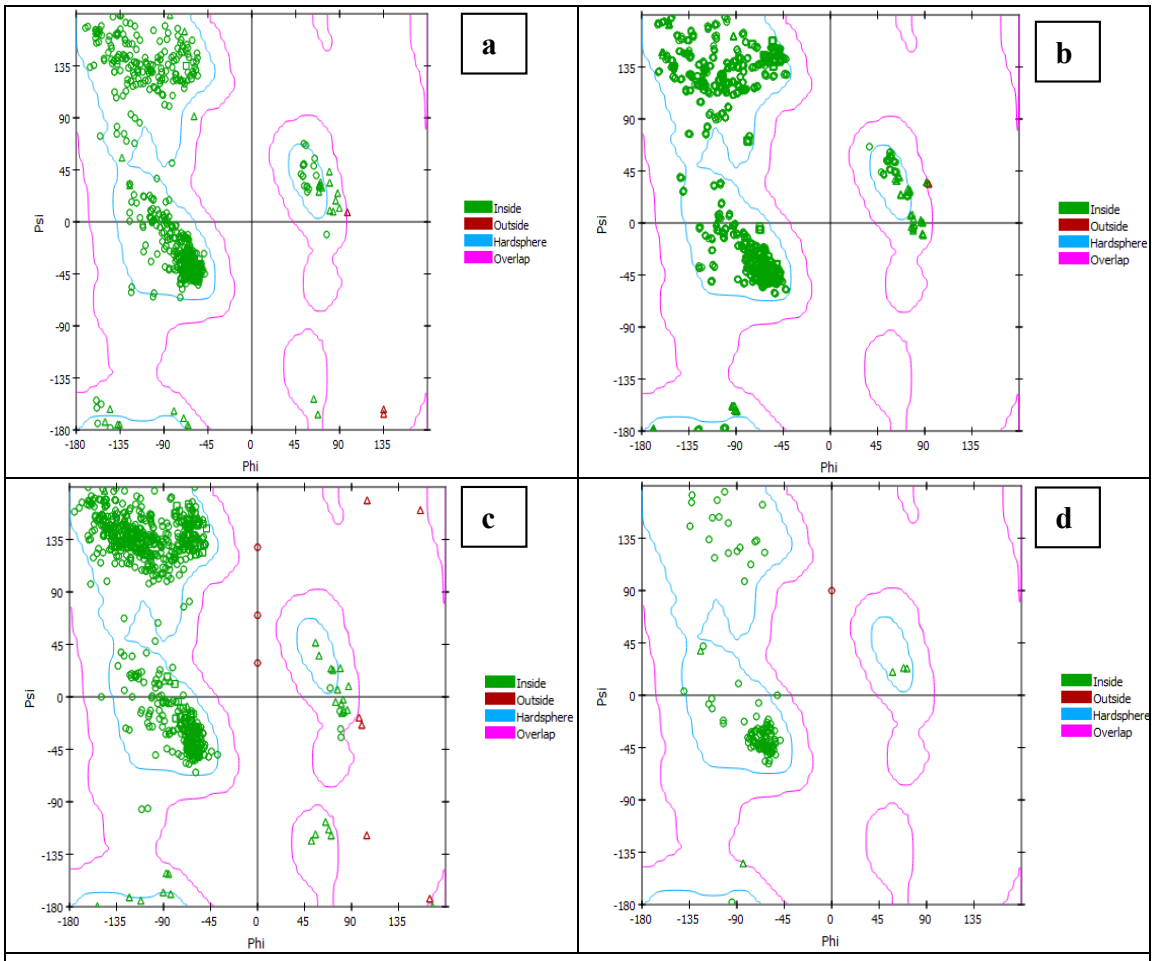


Fig 1: Ramachandran plot of (a) 6LL7 (b) 5NNY (c) 6IZO (d) 5VA4

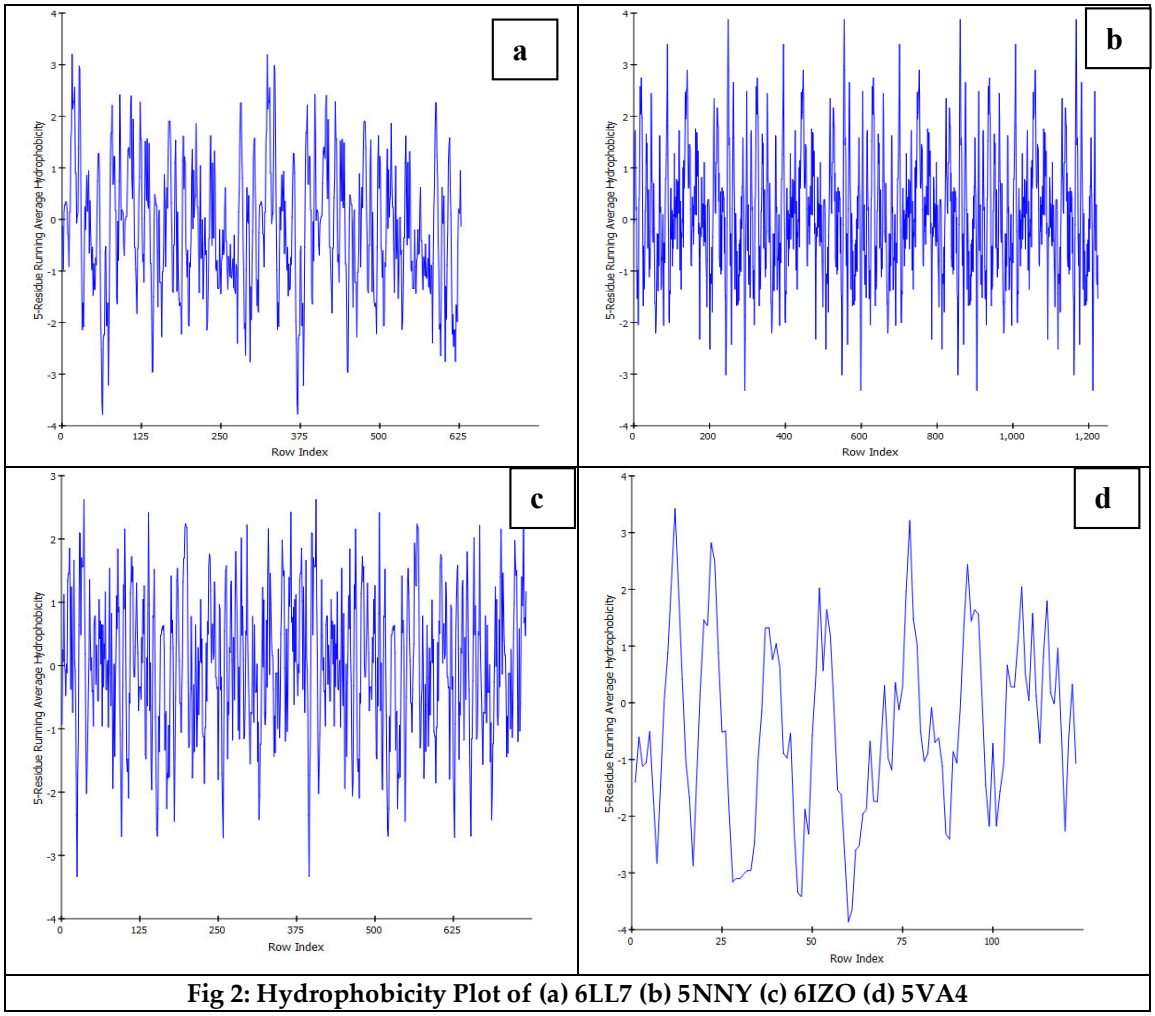
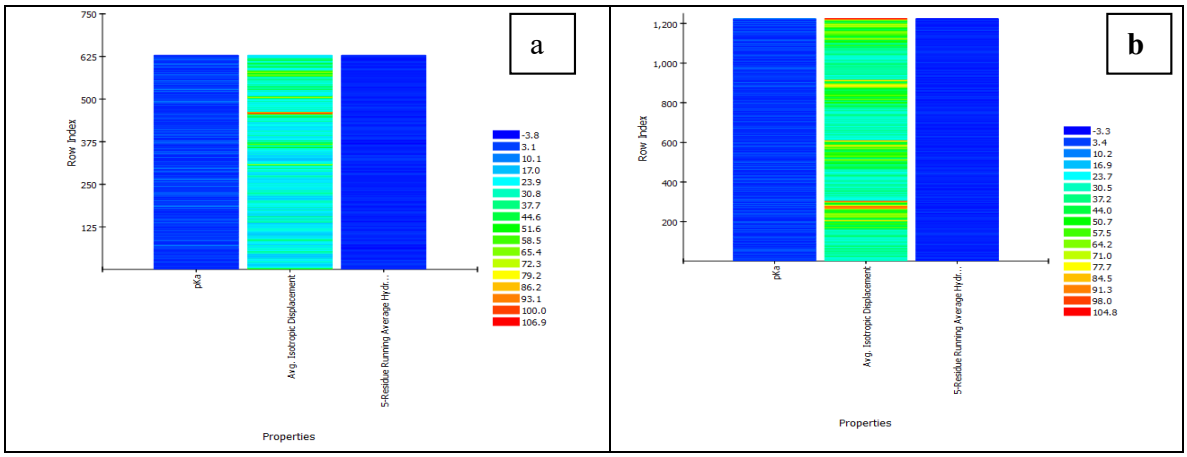


Fig 2: Hydrophobicity Plot of (a) 6LL7 (b) 5NNY (c) 6IZO (d) 5VA4



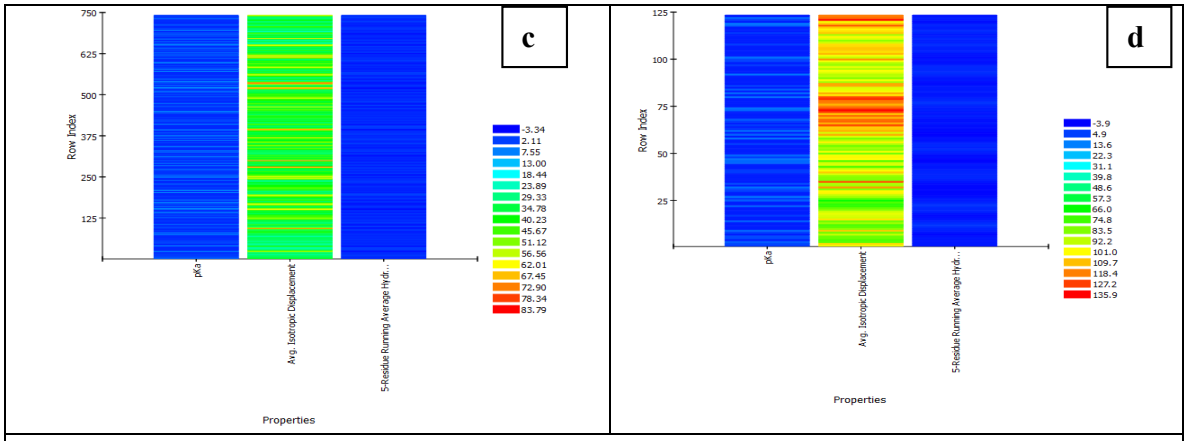
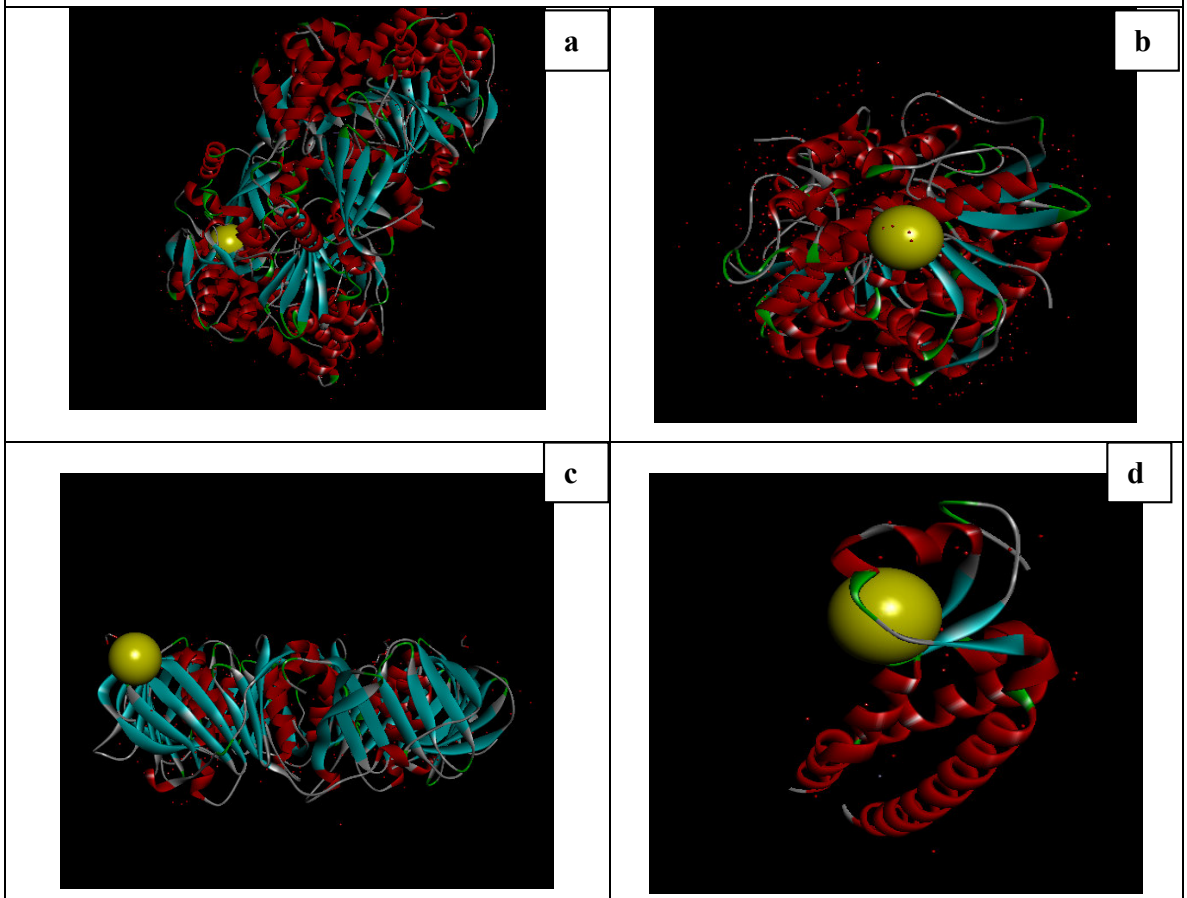


Fig 3: Heat Map Plot of (a) 6LL7 (b) 5NNY (c) 6IZO (d) 5VA4



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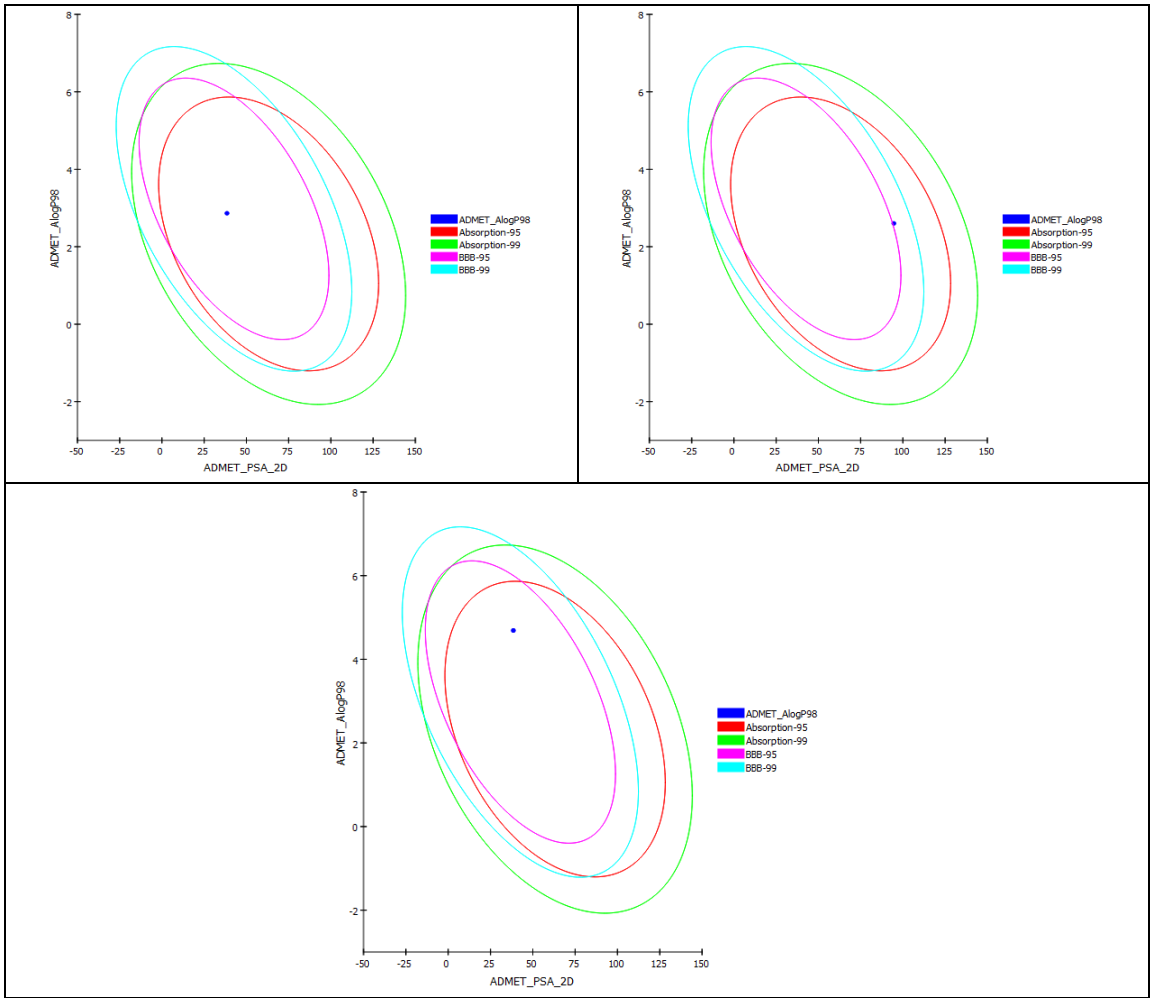

Fig 5: ADMET analysis Report

Table 1: The list of pharmacophores and the targeted genes from Yellow Leaf Curl

Sl. No	Long pepper Pharmacophores	Targeted Plant Disease Causing Microbial (Tomato yellow leaf curl virus)Gene	Pdb
1	Pellitorine	Rep protein	6LL7
2	Piperine	precoat protein	5NNY
3	Pipernonaline	replication initiator protein	6IZO
4	Coumaperine	capsid protein	5VA4

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RESEARCH ARTICLE

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Protein–protein interactions (protein functionalities) are mediated by water, which compacts individual proteins and promotes close and temporarily stable large-area protein–protein interfaces. In their classic article, Kyte and Doolittle (KD) concluded that the "simplicity and graphic nature of hydrophobicity scales make them very useful tools for the evaluation of protein structures." In practice, however, attempts to develop hydrophobicity scales (for example, compatible with classical force fields (CFF) in calculating the energetics of protein folding) have encountered many difficulties.

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ADMET Analysis

Considering the comparable CDOCKER energy, interaction energy and binding energy, three compounds were forwarded for ADMET analysis. These studies are based on the ADMET(Absorption, Distribution, Metabolism, Excretion and Toxicity) properties of the compounds. These properties provide insights in to the pharmacokinetic properties of the compounds and were checked using Discovery Studio's built in ADMET protocol. The various parameters tested in this study were aqueous solubility, Blood Brain Barrier (BBB) level, Hepatotoxicity, Absorption level, AlogP and CYPD26. Pharmacokinetic properties of the best fit phytochemicals showed that two of the compounds had passed all the pharamacokinetic parameters. The compounds that passed the parameters were N-methyltyramine and dalbergioidin. These compounds were thus selected as the best compounds in this study as they had good interaction scores along with ADMET properties.

CONCLUSION

The perceived pharmacophores can be bound from the Long pepper and can be advanced as the normal prescription for the Cholera which is having lesser terrible manifestation from the chemotherapeutic drug open in the market. This medicine will in like manner be amazingly more affordable from the available meds and these meds are also not destructive for the run of the mill cells as they are gotten from the ordinary things.

The stand-out segment of the examination is to centered quality treatment for biopesticides. This will help our future medicine with being completely related to the Pharmachophores and the businesses of produced and malignant growth causing drug will diminish.

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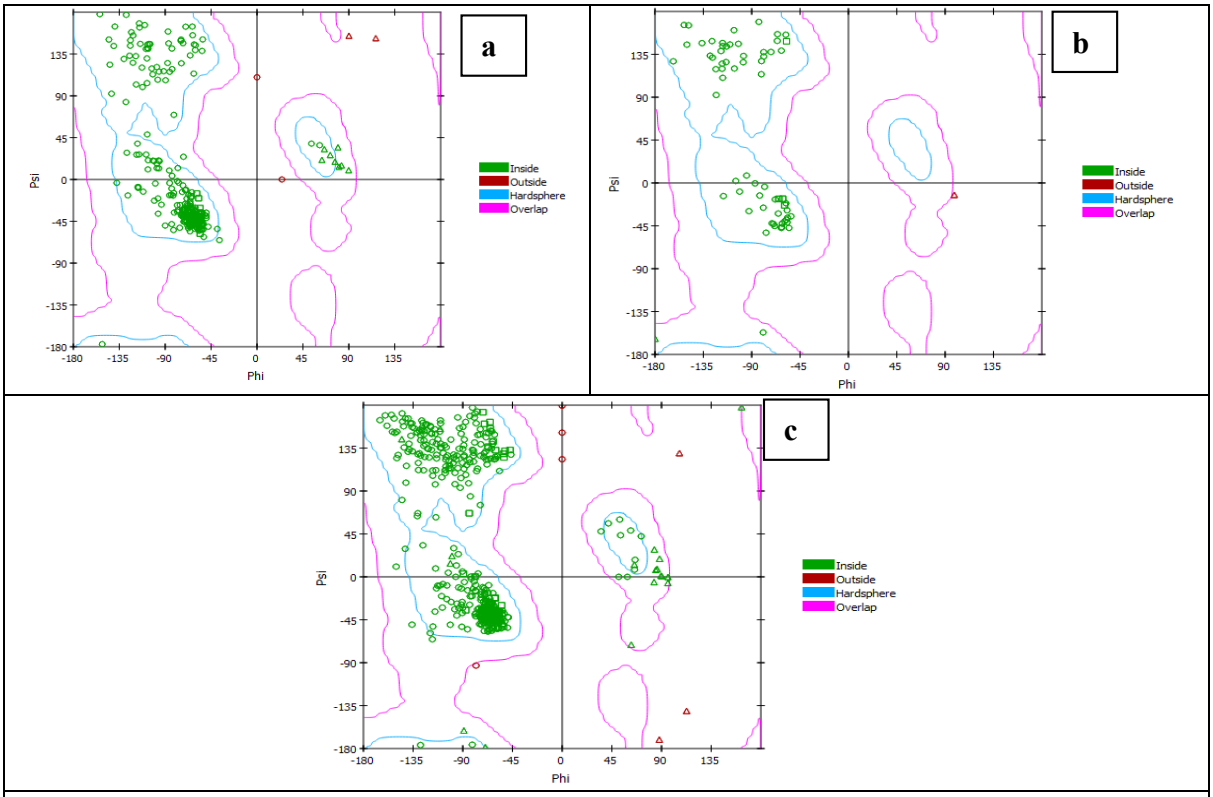
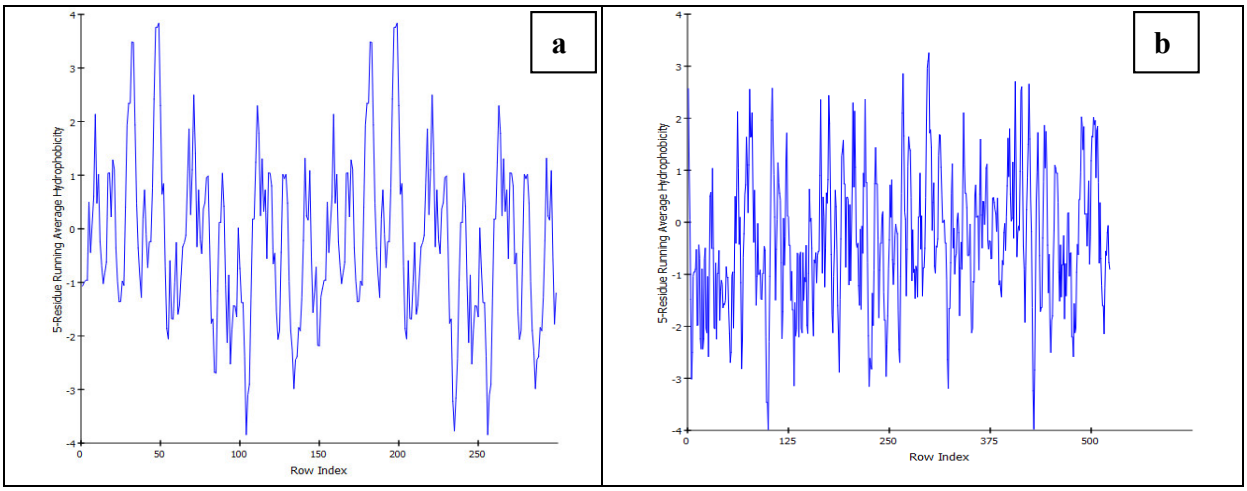


Fig 1: Ramachandran plot of (a) 6NJS (b) 6N2U (c) 3X1O



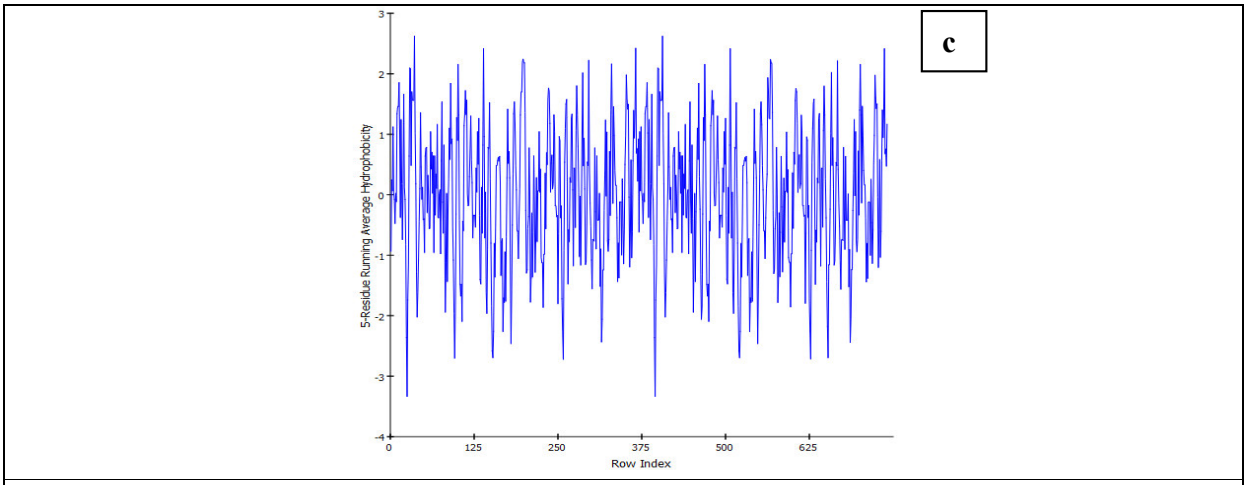


Fig 2: Hydrophobicity Plot of (a) 6NJS (b) 6N2U (c) 3X1O

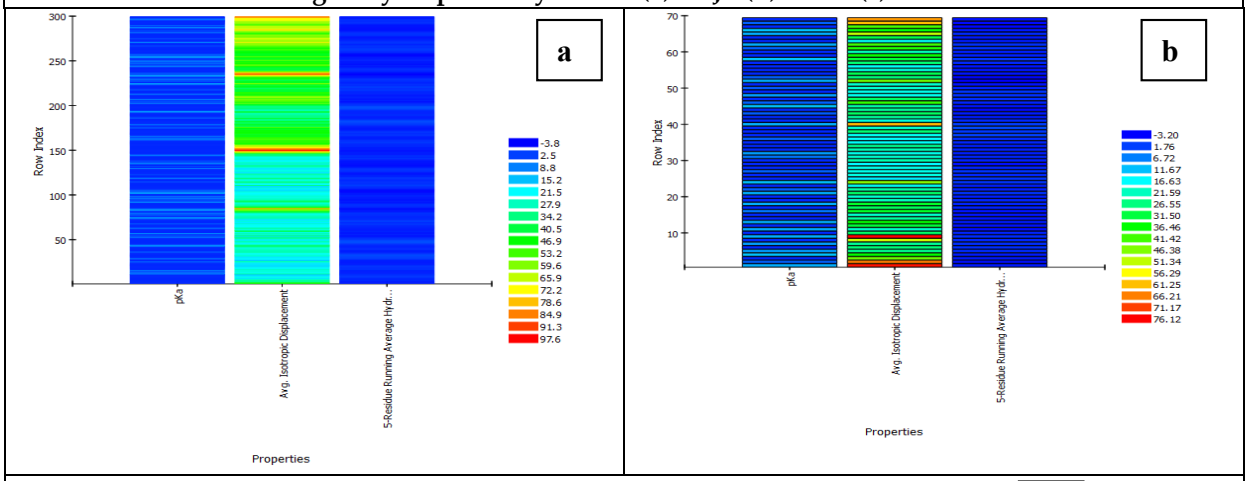


Fig 3: Heatmap Plot of (a) 6NJS (b) 6N2U (c) 3X1O

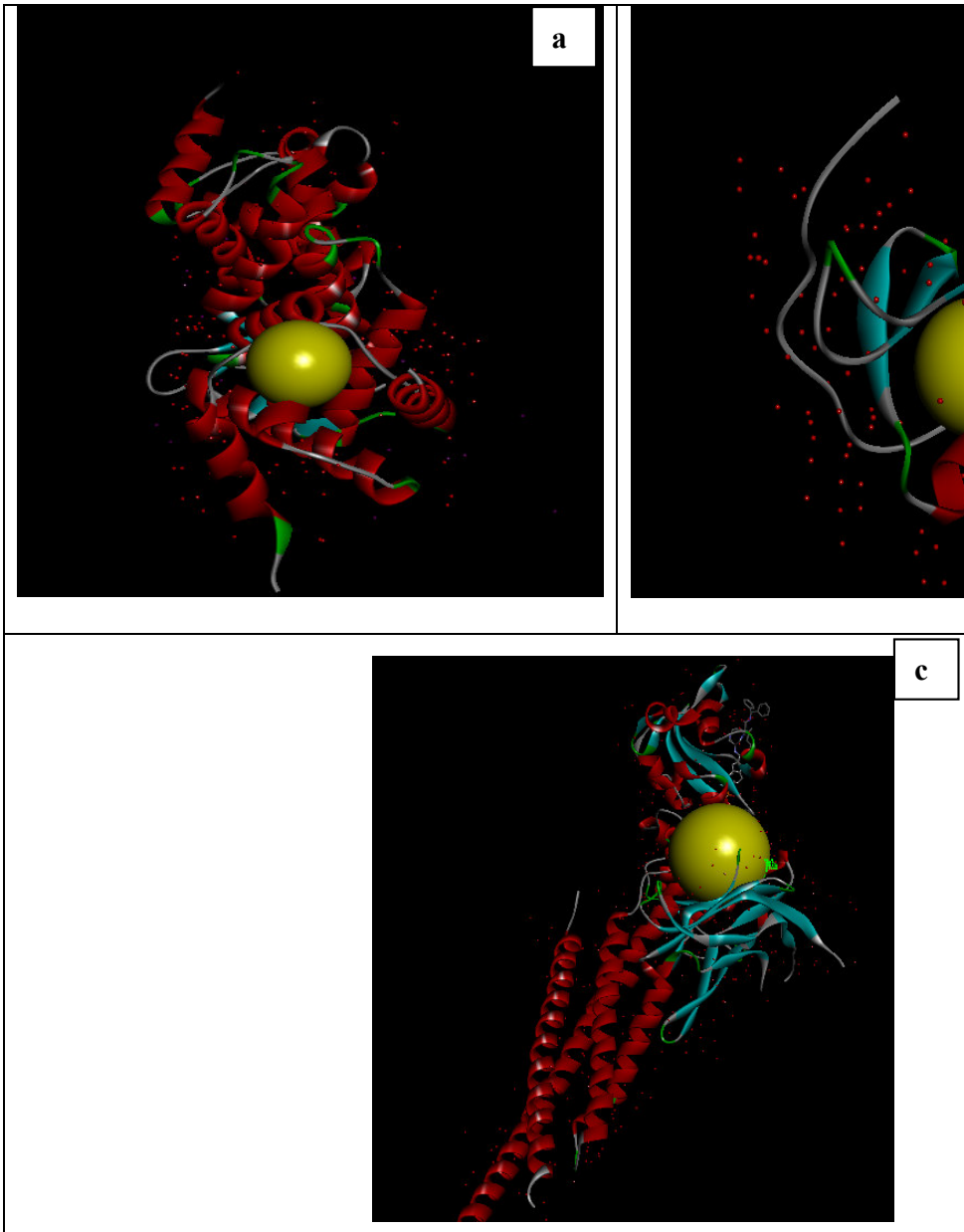


Fig 4: Docking Result of (a) 6NJS (b) 6N2U (c) 3X1O

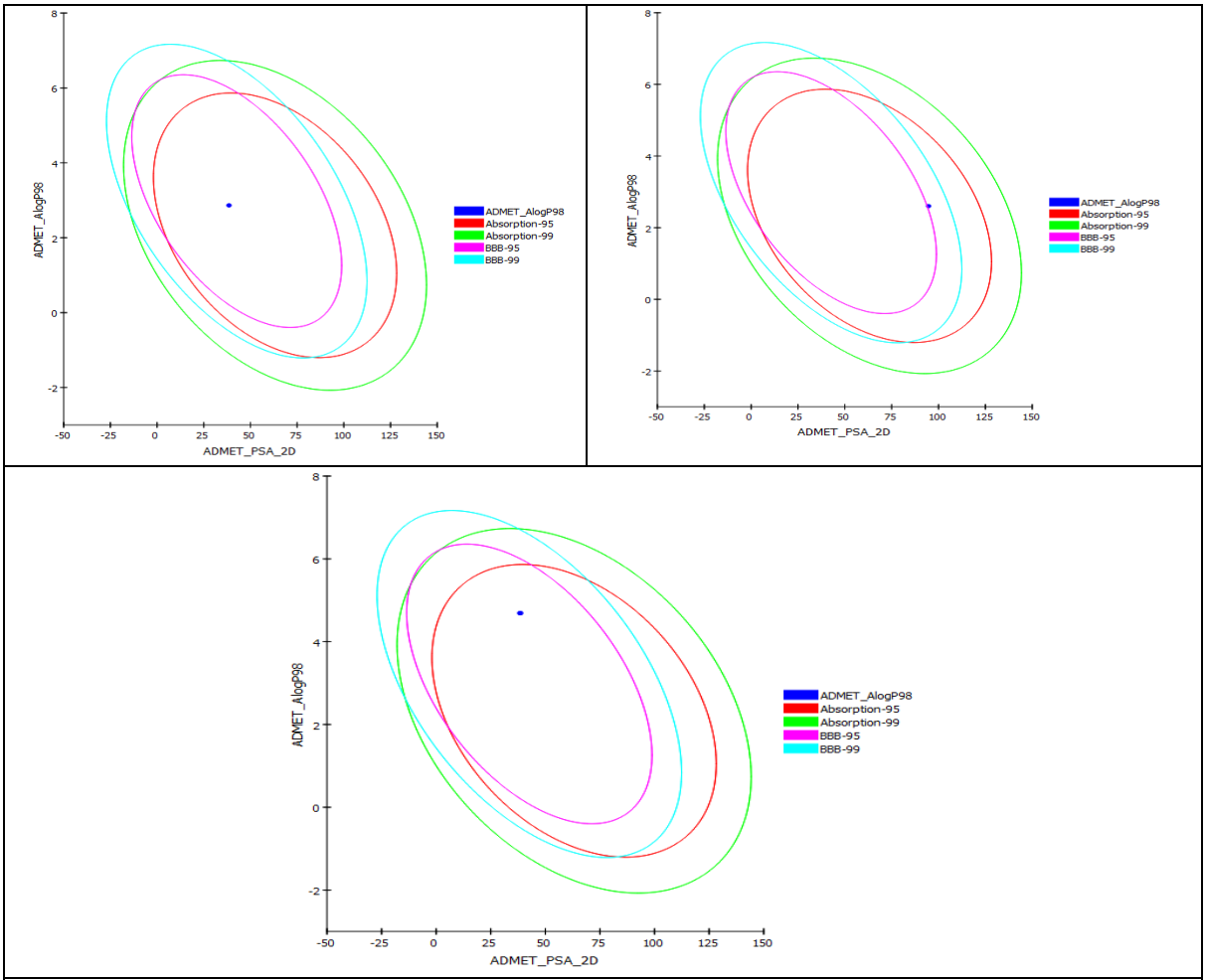


Fig 5: ADMET analysis Report

Table 1: The list of pharmacophores and the targeted genes from Black gram and green gram

Sl. No	Long pepper Pharmacophores	Targeted Animal Gene (Cholera)	PDB No of the Genes
1	Pellitorine	signal transducer and activator of transcription 3	6NJS
2	Piperine	C-X-C motif chemokine ligand 8	6N2U
3	Pipernonaline	microRNA 146a	3X1O
4	Coumaperine	microRNA 155	6N5Q

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RESEARCH ARTICLE

In silico Analysis of the Rosemary as Targeted Therapy for Targeted Animal Disease Nephritis

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ABSTRACT

As native wellsprings of meds, therapeutic plants are utilized from the antiquated occasions. Rosemary is one of the profoundly utilized potential therapeutic plants on the planet. This plant is customarily utilized for the treatment of regular cold, loose bowels, fever because of a few infective reason, jaundice, as a wellbeing tonic for the liver and cardiovascular wellbeing, and as a cancer prevention agent. It is additionally used to improve sexual dysfunctions and fill in as a prophylactic. All pieces of this plant are utilized to separate the dynamic phytochemicals, yet the structures of phyto constituents generally vary starting with one section then onto the next and with spot, season, and time of collect. We are utilizing this property of Rosemary to get some new medications for Nephritis. The employments of different pesticides, additives, and so forth transform the nourishments into poison. Besides the reactions of these pesticides and additives, and so forth are perilous as in light of the fact that it prompts commencement of various malignant growth. In this entire world, the quantity of patients passing on from malignant growth is expanding in a compromising manner. In-silico investigation has done utilizing programming and we further focused on a portion of the qualities liable for Nephritisand pharmacophores from Rosemary and destroyed some silico examination. In this we have discovered that these two pharmacophores are having better Mol Doc score from any others. From this we can find that these two pharmacophores can be an answer for pesticides in not so distant future

Keywords: nephritis, docking, *in silico* analysis, pharmacophore, rosemary

INTRODUCTION

Rosemary (*Rosmarinus officinalis*) is a woody enduring flavor plant and restorative plant local to the Mediterranean bowl and developed in pasty soil. We get sweet-smelling oil from stems, leaves and blossoms of rosemary. it's generally utilized as a food additive and sauce. R. officinalis L. is comprised of bioactive particles, the phytocompounds, liable for actualize a few pharmacological exercises, as antitumor, cancer prevention agent, mitigating, antimicrobial, antiproliferative, and defensive, constricting and inhibitory exercises. The utilization of rosemary separate as a characteristic cancer prevention agent was first revealed in 1955.

Rosemary includes a rich history, holding a unique situation among herbs for the imagery associated with it. In Europe rosemary includes an extremely old notoriety for improving memory, and has been utilized as a logo of fellowship, reliability and for recognition during weddings, war celebrations and memorial services (Moss, 2003). In old Greece, understudies would put rosemary branches in their hair to upgrade memory and fixation when reading for assessment (Calucci et al., 2003). Rosemary leaves are singed as an incense, fumigant and disinfectant, in times past, the herb was scorched in wiped out chambers to cleanse the air and was put in law courts as an insurance from prison fever (typhus), and through the Plague of 1665, and rosemary was conveyed and sniffed in dubious territories to ensure against plague. Strengthening those germ-free uses, a blend of rosemary and juniper was singed during war II in French medical clinics to eliminate germs (Usher, 1974; Phillips and Foy, 1990). In old China, rosemary was utilized for cerebral pains, a sleeping disorder, and mental exhaustion and topically for hairlessness (Leung and Foster, 1996). In India, rosemary appreciates a past filled with use as an energizer and as a carminative to remove gas from the stomach and digestive organs and as antimigraine (Nadkarni, 1994). The Egyptians utilized the plant for incense in custom purifying and mending. Anthropologists and archeologists have discovered proof that rosemary herbs were utilized as restorative, culinary and beautifying agents temperances inside the old Egypt, Mesopotamia, China and India (Stefanovits-Banyai et al., 2003) eliminate germs (Usher, 1974; Phillips and Foy, 1990). This medicinalR. officinalis plant is comparing to certain phytochemicals, for example, caffeic corrosive, carnosic corrosive, chlorogenic corrosive, monomeric corrosive, oleanolic corrosive, rosmarinic corrosive, rosmaquinones An and B , alpha-pinene , rosmanol , carnosol, ursolic corrosive, secohinokio, camphor, eucalyptol, rosmadial, and subsidiaries of eugenol and luteolin. The impacts showed by this plant incorporate (1) avoidance of issues related with atherosclerosis; (2) anticancer and antiproliferative impacts; (3) antiulcer activity ; (4) myocardial indispensable sign decrease with rosmarinic corrosive ; (5) cell reinforcement and calming activities of rosmarinic corrosive; (6) lipid peroxidation decrease in heart and cerebrum; (7) antiangiogenic and neuroprotective impacts of carnosic corrosive and carnosol; (8)ability to constrict asthma, atherosclerosis, waterfall, torment , hepatotoxicity, peptic ulceration , incendiary ailments, ischemic coronary illness; (9) control of hypercholesterolemia and oxidative pressure and help of physical and mental weakness; (10) antiviral; and antimicrobial activities ; (11) glycemia decrease , nephroprotective and radioprotective-antimutagenic limits; (12) hepatoprotective; (13) capacity to treat burdensome conduct; (14) relaxant and treatment for cutaneous sensitivity.

MATERIAL AND METHODS

Phytochemicals of Rosemary have been listed with their structure data files which are taken from pubchem ChEBI. Genes has been taken randomly for Nephritisusing NCBI database. Table 1 has been showing the enlisted pharmacophores and the targeted genes. The PDB numbers of gene are taken from RCSB. The In-silico analysis has been done using BIOVIA –Discovery studio. We have performed various docking and used the Ramachandran plot and others.

Protein identification and preparation

The announced atomic targets liable for Nephritisare taken (Table 1) and the X-beam crystallographic structures of these objective proteins were recovered from protein information bank (PDB). The recovered PDB structures contain water particles, substantial iotas, cofactors, metal particles and so forth and these structures don't have data about topologies, bond requests and formal nuclear charges. Thus the downloaded PDB structures were readied utilizing 'plan protein' convention of Discovery Studio 4.0. The objective proteins were set up by evacuating all water particles, ligands and other hetero molecules from the structures. Hydrogen iotas were added to the particles to fulfill their valencies. The structures were then vitality limited by applying CHARM power field to evacuate the steric conflicts between the molecules so as to get steady adaptation.

Active site identification

The binding sites of the receptor proteins were predicted based on 'receptor cavity method' using Accelry's Discovery Studio 4.0. Using this protocol, active sites of the target receptor were identified based upon the inhibitory property of the amino acid residues present in the binding sites.

Ligand preparation and filtration

An arrangement of 4 phyto blends from Rosemary was taken as ligands for docking examination. The 3D structures of these blends were downloaded from PubChem database. These ligands were then cleaned up, decided 3D encourages and made ligand adjustments by applying 'plan ligand show' of Discovery Studio 4.0. After preparation, the blends were isolated reliant on the nuclear properties for predicting their dissolvability and vulnerability in sedate divulgence. The most mainstream of the physical property channels is Lipinski's "rule-offive", which revolves around bioavailability. The standard communicates that the blends have nuclear mass under 500 daltons, not more than 5 hydrogen security advocates, not more than 10 hydrogen security acceptors and an octanol-water section coefficient log P not more unmistakable than 5 (Lipinski et al.,2001). The filtered blends were then used for docking assessment.

Docking

The antimicrobial action of all the 4 phytochemicals detailed from Rosemary was evaluated by docking these mixes against the particular dynamic locales of the objective proteins. Disclosure studio 4.0 was utilized in this examination to discover the collaborating mixes of Rosemary with the chose focuses of joint pain. Techniques of Discovery Studio 4.0 are to thoroughly dock or score potential places of every ligand in the coupling site of the proteins. Docking investigation of the objective proteins was finished with common mixes got from Rosemary to locate the favored direction and restricting fondness of the mixes with each target protein utilizing scoring capacities. A sub-atomic elements (MD) reproduced toughening based calculation, specifically, CDOCKER was utilized to score the associating mixes. This strategy utilizes a gridbased portrayal of the protein-ligand potential connections to figure the coupling fondness (Wu et al., 2003). CDOCKER utilizes delicate center possibilities, which are seen as successful in the age of a few irregular adaptations of little organics and macromolecules inside the dynamic site of the objective protein. Ligands were docked to the proteins followed by scoring them for their overall quality of cooperation to distinguish possibility for tranquilize advancement. The last stances were then scored dependent on the absolute docking vitality, which is made out of intramolecular vitality of ligand and the ligand-protein association. The most minimal vitality structure was taken as the best fit. Understanding of the qualities was finished utilizing measures gave by Discovery Studio, for example, CDOCKER vitality, CDOCKER collaboration vitality, hydrogen bonds, restricting vitality and so on.

Drug likeliness

Drug-likeness is a qualitative concept used in drug design to evaluate how the substance acts like drug with respect to factors like bioavailability. The molecular properties which influence absorption, distribution, metabolism, excretion and toxicity are recognized as a long side therapeutic potency as key determinants of whether a molecule can be successfully developed as a drug (Zhang et al., 2012). These parameters are responsible for about 60 percent failures of all drugs in the clinical phases and so the prediction of ADMET properties plays a significant role in new drug discovery process (Hire et al., 2012). Thus, it has become imperative to design lead compounds which would be easily Breast ly absorbed, easily transported to their targeted site of action, not easily converted into toxic metabolic products and easily eliminated from the body before accumulating in sufficient amounts. The ADMET properties of the compounds were analyzed for drug like candidates.

RESULT AND DISCUSSION

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The three dimensional structures of the identified target proteins were retrieved from the protein data bank. PDB ID of the targeted protein structure are mentioned in Table 1.

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CONCLUSION

The recognized pharmacophores can be confined from the Rosemary and can be popularized as the common medication for the Nephritis which is having lesser hurtful symptom from the chemotherapeutic medication accessible in the market. This medication will likewise be extremely less expensive from the accessible medications and these medications are additionally not hurtful for the typical cells as they are gotten from the normal items. The one of a kind component of the investigation is to focus quality treatment for targeted drug. This will assist our future medication with being totally associated to the Pharmachophores and the employments of manufactured and cancer-causing medication will decrease.

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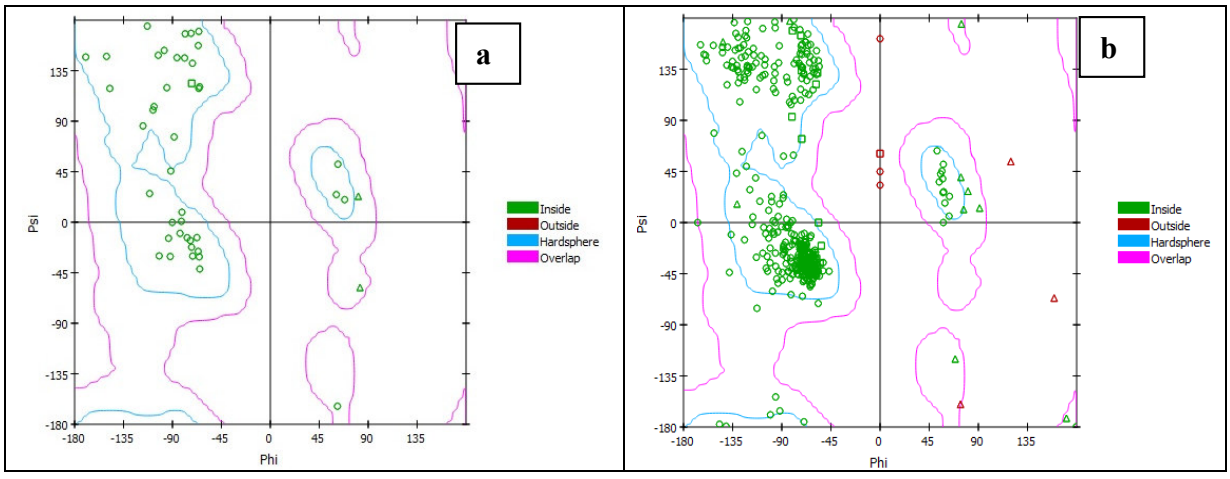

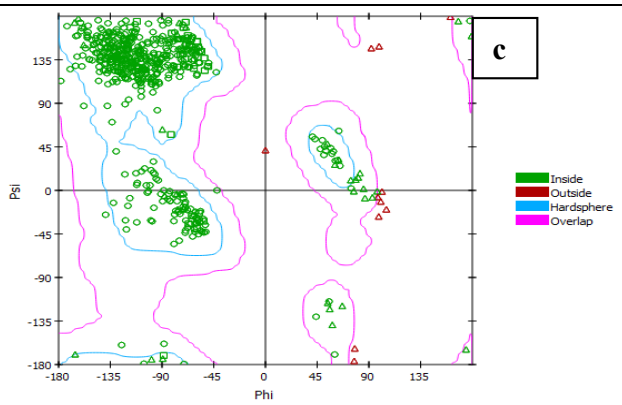

Fig 1: Ramachandran plot of (a) 2M0P (b) 5HVQ (c) 6TT1

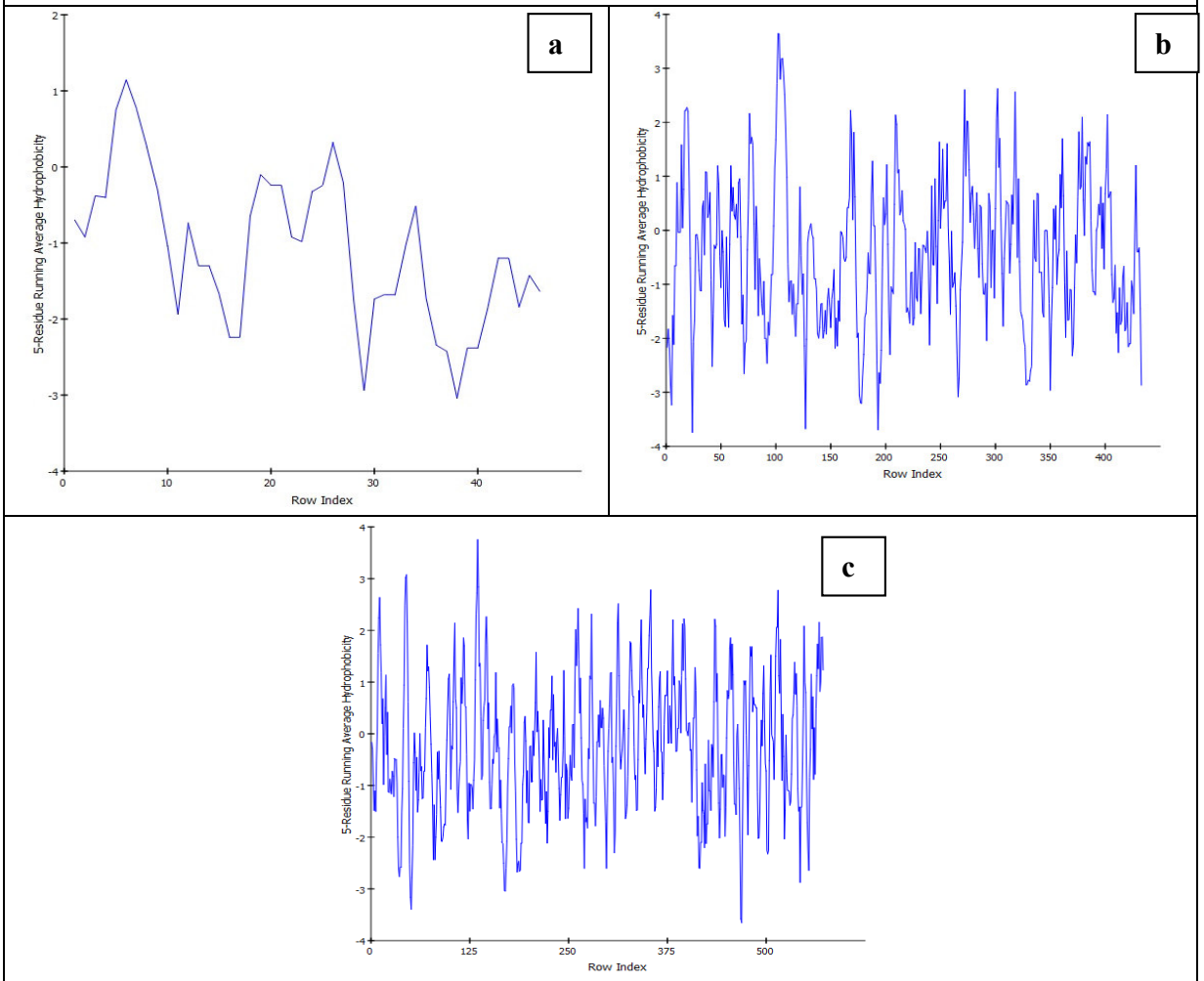

Fig 2: Hydrophobicity Plot of (a) 2M0P (b) 5HVQ (c) 6TT1

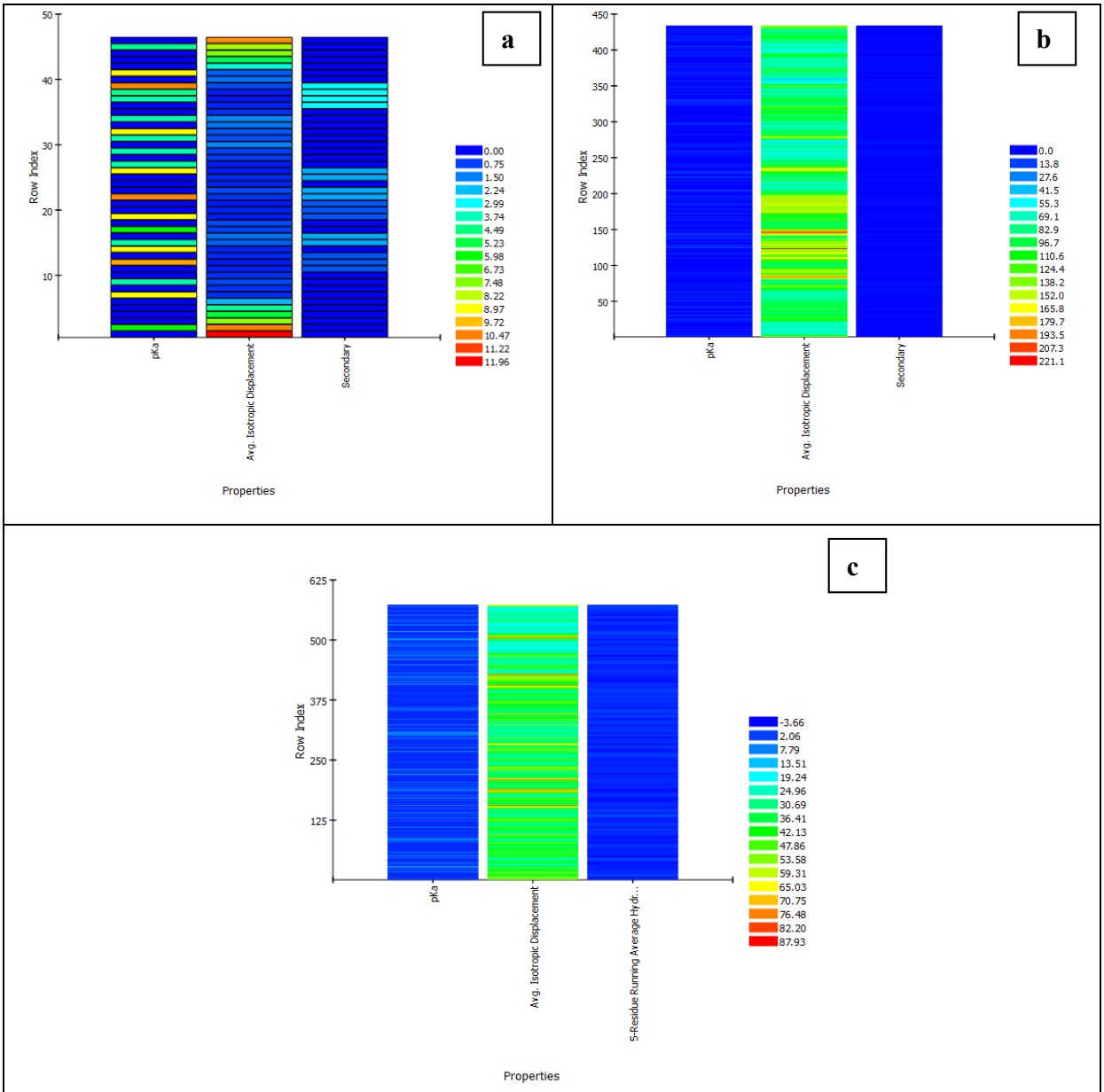

Fig 3: Heatmap Plot of (a) 2M0P (b) 5HVQ (c) 6TT1

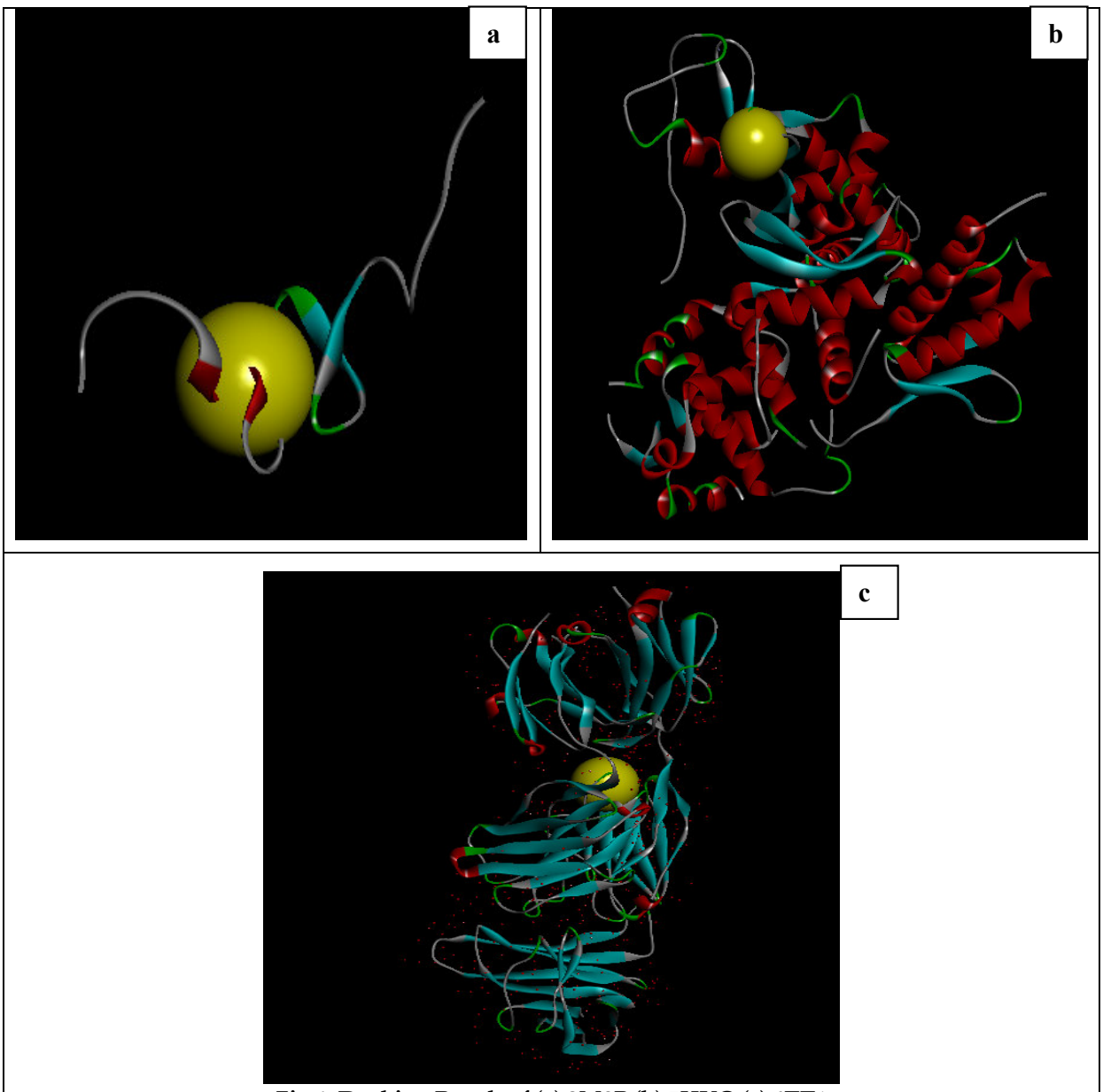

Fig 4: Docking Result of (a) 2M0P (b) 5HVQ (c) 6TT1

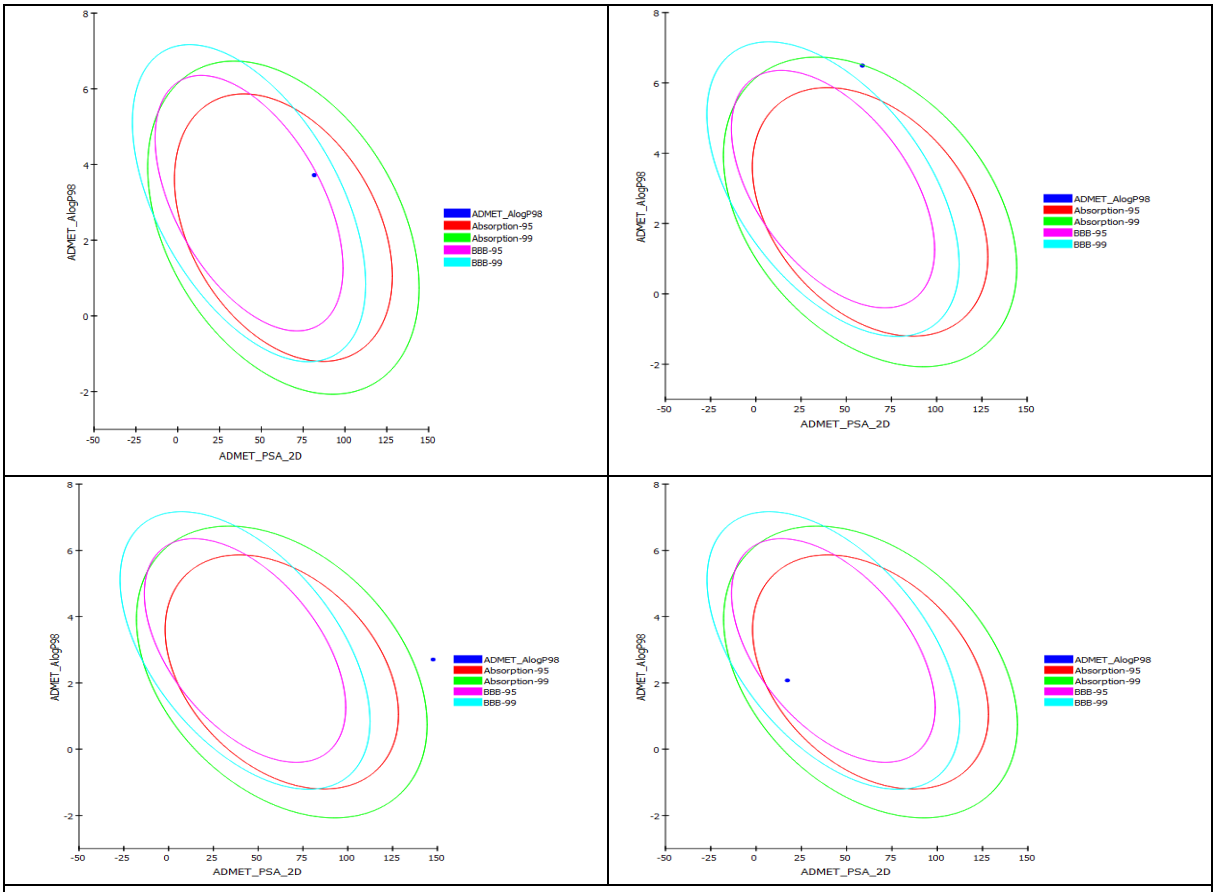

Fig 5: ADMET analysis Report

Table 1: The list of pharmacophores and the targeted genes from Nephitis

Sl. No	Pharmacophores from Rosemary	Targeted Animal Gene (Nephritis)	PDB No of the Genes
1	Rosemerinic acid	LDL receptor related protein 2	2M0P
2	Ursolic acid	tubulointerstitial nephritis antigen	5HVQ
3	Camphor	angiotensin I converting enzyme	6TT1
4	Rosmadial		

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RESEARCH ARTICLE

In silico Analysis of the Rosemary as Targeted Therapy for Targeted Plant Disease Causing Microbial Disease Black Gram and Green Gram

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ABSTRACT

As native wellsprings of drugs, restorative plants are utilized from the antiquated occasions. Rosemary is one of the exceptionally utilized potential therapeutic plants on the planet. This plant is generally utilized for the treatment of basic cold, loose bowels, fever because of a few infective reason, jaundice, as a wellbeing tonic for the liver and cardiovascular wellbeing, and as a cancer prevention agent. It is additionally used to improve sexual dysfunctions and fill in as a prophylactic. All pieces of this plant are utilized to separate the dynamic phytochemicals, however the arrangements of phytoconstituents generally vary starting with one section then onto the next and with spot, season, and time of gather. We are utilizing this property of Rosemary to get some new medications for Black gram and green gram. The employments of different pesticides, additives, and so on transform the nourishments into poison. Also the symptoms of these pesticides and additives, and so on are perilous as in light of the fact that it prompts commencement of various malignant growth. In this entire world, the quantity of patients biting the dust from malignancy is expanding in a compromising manner. In-silico investigation has done utilizing programming and we further focused on a portion of the qualities liable for Black gram and green gram and pharmacophores from Rosemary and destroyed some silico examination. In this we have discovered that these two pharmacophores are having better Mol Doc score from any others. From this we can reason that these two pharmacophores can be an answer for pesticides in not so distant future.

Keywords: black gram and green gram, docking, *in silico* analysis, pharmacophore, rosemary

INTRODUCTION

Rosemary (*Rosmarinus officinalis*) is a woody perennial spice plant and medicinal plant native to the Mediterranean basin and grown in chalky soil. We get aromatic oil from stems, leaves and flowers of rosemary. it's commonly used as a food preservative and condiment. R. officinalis L. is made up of bioactive molecules, the phytocompounds, responsible for implement several pharmacological activities, like antitumor, antioxidant, anti-inflammatory, antimicrobial, antiproliferative, and protective, attenuating and inhibitory activities. theutilization of rosemary extract as a natural antioxidant was first reported in 1955. Rosemary features a rich history, holding a special position among herbs for the symbolism connected with it. In Europe rosemary features a very old reputation for improving memory, and has been used as a logo of friendship, loyalty and for remembrance during weddings, war commemorations and funerals (Moss, 2003). In ancient Greece, students would place rosemary sprigs in their hair to enhance memory and concentration when studying for examination (Calucci et al., 2003). Rosemary leaves are burnt as an incense, fumigant and disinfectant, in times past, the herb was burned in sick chambers to purify the air and was placed in law courts as a protection from jail fever (typhus), and through the Plague of 1665, and rosemary was carried and sniffed in suspicious areas to protect against plague. Reinforcing those antiseptic uses, a mix of rosemary and juniper was burned during war II in French hospitals to kill germs (Usher, 1974; Phillips and Foy, 1990). In ancient China, rosemary was used for headaches, insomnia, and mental fatigue and topically for baldness (Leung and Foster, 1996). In India, rosemary enjoys a history of use as a stimulant and as a carminative to expel gas from the stomach and intestines and as antimigraine (Nadkarni, 1994). The Egyptians used the plant for incense in ritual cleansing and healing. Anthropologists and archaeologists have found evidence that rosemary herbs were used as medicinal, culinary and cosmetics virtues within the ancient Egypt, Mesopotamia, China and India (Stefanovits-Banyai et al., 2003) kill germs (Usher, 1974; Phillips and Foy, 1990). This medicinal *R. officinalis* plant is corresponding to some phytochemicals such as caffeic acid, carnosic acid, chlorogenic acid, monomeric acid, oleanolic acid, rosmarinic acid, rosmaquinones A and B , alpha-pinene , rosmanol , carnosol, ursolic acid, secohinokio, camphor, eucalyptol, rosmadial, and derivatives of eugenol and luteolin. The effects demonstrated by this plant include (1) prevention of problems associated with atherosclerosis; (2) anticancer and antiproliferative effects; (3) antiulcer action ; (4) myocardial vital sign reduction with rosmarinic acid ; (5) antioxidant and anti-inflammatory actions of rosmarinic acid; (6) lipid peroxidation reduction in heart and brain; (7) antiangiogenic and neuroprotective effects of carnosic acid and carnosol; (8)ability to attenuate asthma, atherosclerosis, cataract, pain , hepatotoxicity, peptic ulceration , inflammatory diseases, ischemic heart disease; (9) control of hypercholesterolemia and oxidative stress and relief of physical and mental fatigue; (10) antiviral; and antimicrobial actions ; (11) glycemia reduction , nephroprotective and radioprotective-antimutagenic capacities; (12) hepatoprotective; (13) ability to treat depressive behaviour; (14) relaxant and treatment for cutaneous allergy.

MATERIAL AND METHODS

Phytochemicals of Rosemary have been listed with their structure data files which are taken from pubchem ChEBI. Genes has been taken randomly for Black gram and green gram using NCBI database. Table 1 has been showing the enlisted pharmacophores and the targeted genes. The PDB numbers of gene are taken from RCSB. The In-silico analysis has been done using BIOVIA –Discovery studio. We have performed various docking and used the Ramachandran plot and others.

Protein identification and preparation

The reported molecular targets responsible for Black gram and green gram are taken (Table 1) and the X-ray crystallographic structures of these target proteins were retrieved from protein data bank (PDB). The retrieved PDB structures contain water molecules, heavy atoms, cofactors, metal ions etc. and these structures do not have information about topologies, bond orders and formal atomic charges. Hence the downloaded PDB structures were

prepared using 'prepare protein' protocol of Discovery Studio 4.0. The target proteins were prepared by removing all water molecules, ligands and other hetero atoms from the structures. Hydrogen atoms were added to the atoms to satisfy their valencies. The structures were then energy minimized by applying CHARM force field to remove the steric clashes between the atoms in order to get stable conformation.

Active site identification

The binding sites of the receptor proteins were predicted based on 'receptor cavity method' using Accelry's Discovery Studio 4.0. Using this protocol, active sites of the target receptor were identified based upon the inhibitory property of the amino acid residues present in the binding sites.

Ligand preparation and filtration

An assortment of 4 phyto mixes from Rosemary was taken as ligands for docking investigation. The 3D structures of these mixes were downloaded from PubChem database. These ligands were then tidied up, determined 3D facilitates and created ligand adaptations by applying 'plan ligand convention' of Discovery Studio 4.0. After readiness, the mixes were separated dependent on the atomic properties for foreseeing their dissolvability and penetrability in medicate disclosure. The most popular of the physical property channels is Lipinski's "rule-offive", which centers around bioavailability. The standard expresses that the mixes have atomic mass under 500 daltons, not in excess of 5 hydrogen bond benefactors, not in excess of 10 hydrogen bond acceptors and an octanol-water segment coefficient log P not more prominent than 5 (Lipinski et al.,2001). The sifted mixes were then utilized for docking examination.

Docking

The antimicrobial action of all the 4 phytochemicals detailed from Rosemary was evaluated by docking these mixes against the particular dynamic locales of the objective proteins. Disclosure studio 4.0 was utilized in this examination to discover the collaborating mixes of Rosemary with the chose focuses of joint pain. Techniques of Discovery Studio 4.0 are to thoroughly dock or score potential places of every ligand in the coupling site of the proteins. Docking investigation of the objective proteins was finished with common mixes got from Rosemary to locate the favored direction and restricting fondness of the mixes with each target protein utilizing scoring capacities. A sub-atomic elements (MD) reproduced toughening based calculation, specifically, CDOCKER was utilized to score the associating mixes. This strategy utilizes a gridbased portrayal of the protein-ligand potential connections to figure the coupling fondness (Wu et al., 2003). CDOCKER utilizes delicate center possibilities, which are seen as successful in the age of a few irregular adaptations of little organics and macromolecules inside the dynamic site of the objective protein. Ligands were docked to the proteins followed by scoring them for their overall quality of cooperation to distinguish possibility for tranquilize advancement. The last stances were then scored dependent on the absolute docking vitality, which is made out of intramolecular vitality of ligand and the ligand-protein association. The most minimal vitality structure was taken as the best fit. Understanding of the qualities was finished utilizing measures gave by Discovery Studio, for example, CDOCKER vitality, CDOCKER collaboration vitality, hydrogen bonds, restricting vitality and so on.

Drug likeliness

Drug-likeness is a qualitative concept used in drug design to evaluate how the substance acts like drug with respect to factors like bioavailability. The molecular properties which influence absorption, distribution, metabolism, excretion and toxicity are recognized as a long side therapeutic potency as key determinants of whether a molecule can be successfully developed as a drug (Zhang et al., 2012). These parameters are responsible for about 60 percent failures of all drugs in the clinical phases and so the prediction of ADMET properties plays a significant role in new drug discovery process (Hire et al., 2012). Thus, it has become imperative to design lead compounds which would be easily Breast ly absorbed, easily transported to their targeted site of action, not easily converted into toxic metabolic products and easily eliminated from the body before accumulating in sufficient amounts. The ADMET properties of the compounds were analyzed for drug like candidates.

RESULT AND DISCUSSION

Protein preparation and active site identification

The three dimensional structures of the identified target proteins were retrieved from the protein data bank. PDB ID of the targeted protein structure are mentioned in Table 1.

Ramachandran Plot of the targeted gene

The Ramachandran plot is among the most central concepts in structural biology, seen in publications and textbooks alike. However, with the increasing numbers of known proteinstructures and greater accuracy of ultra-high resolution protein structures, we are still learning more about the basic principles of protein structure. The use of torsion angles to describe polypeptide and protein conformation was developed by Sasisekharan as part of his studies of the structure of collagen chains during his work as a graduate student in the research group of G.N. Ramachandran. The power of this approach was readily apparent and its use quickly became widespread. Using revised definitions, this so-called Ramachandran plot or φ, ψ-plot has remained nearly unchanged in the ensuing fifty years and continues to be an integral tool for protein structure research and education.

Hydrophobicity Plot of the Genes:

Protein–protein interactions (protein functionalities) are mediated by water, which compacts individual proteins and promotes close and temporarily stable large-area protein–protein interfaces. In their classic article, Kyte and Doolittle (KD) concluded that the "simplicity and graphic nature of hydrophobicity scales make them very useful tools for the evaluation of protein structures." In practice, however, attempts to develop hydrophobicity scales (for example, compatible with classical force fields (CFF) in calculating the energetics of protein folding) have encountered many difficulties.

Ligand preparation

4 of the pharmacophores are fulfilled Lipinski rule and are relied upon to be dynamic mixes after Breast organization. The ligand particles with least restricting vitality are considered as mixes with most noteworthy restricting liking. This coupling proclivity showed an engaged collaboration between the above mixes with the objectives contrasted with others. The parameters for finding the best inhibitors, for example, CDOCKER vitality, CDOCKER cooperation vitality and number of hydrogen bonds were additionally assessed. CDOCKER vitality is the joined vitality delivered by the entirety of inward ligand strain vitality and receptor-ligand collaboration vitality where, CDOCKER cooperation vitality is the association vitality between the protein and ligand and the estimations of these two parameters show the quality of communication between the proteins and the ligands. Other than least restricting vitality, mixes with least nuclear vitality distinction between CDOCKER vitality and CDOCKER collaboration vitality were dissected. In view of CDOCKER vitality and CDOCKER collaboration vitality, Fig 4 is indicating the outcome.

ADMET Analysis:

Considering the comparable CDOCKER energy, interaction energy and binding energy, three compounds were forwarded for ADMET analysis. These studies are based on the ADMET(Absorption, Distribution, Metabolism, Excretion and Toxicity) properties of the compounds. These properties provide insights in to the pharmacokinetic properties of the compounds and were checked using Discovery Studio's built in ADMET protocol. The various parameters tested in this study were aqueous solubility, Blood Brain Barrier (BBB) level, Hepatotoxicity, Absorption level, AlogP and CYPD26. Pharmacokinetic properties of the best fit phytochemicals showed that two of the compounds had passed all the pharamacokinetic parameters. The compounds that passed the parameters were N-methyltyramine and dalbergioidin. These compounds were thus selected as the best compounds in this study as they had good interaction scores along with ADMET properties.

CONCLUSION

The recognized pharmacophores can be confined from the Rosemary and can be popularized as the common medication for the Black gram and green gram which is having lesser hurtful symptom from the chemotherapeutic medication accessible in the market. This medication will likewise be extremely less expensive from the accessible medications and these medications are additionally not hurtful for the typical cells as they are gotten from the normal items.

The one of a kind component of the investigation is to focused quality treatment for biopesticides. This will assist our future medication with being totally associated to the Pharmachophores and the employments of manufactured and cancer-causing medication will decrease.

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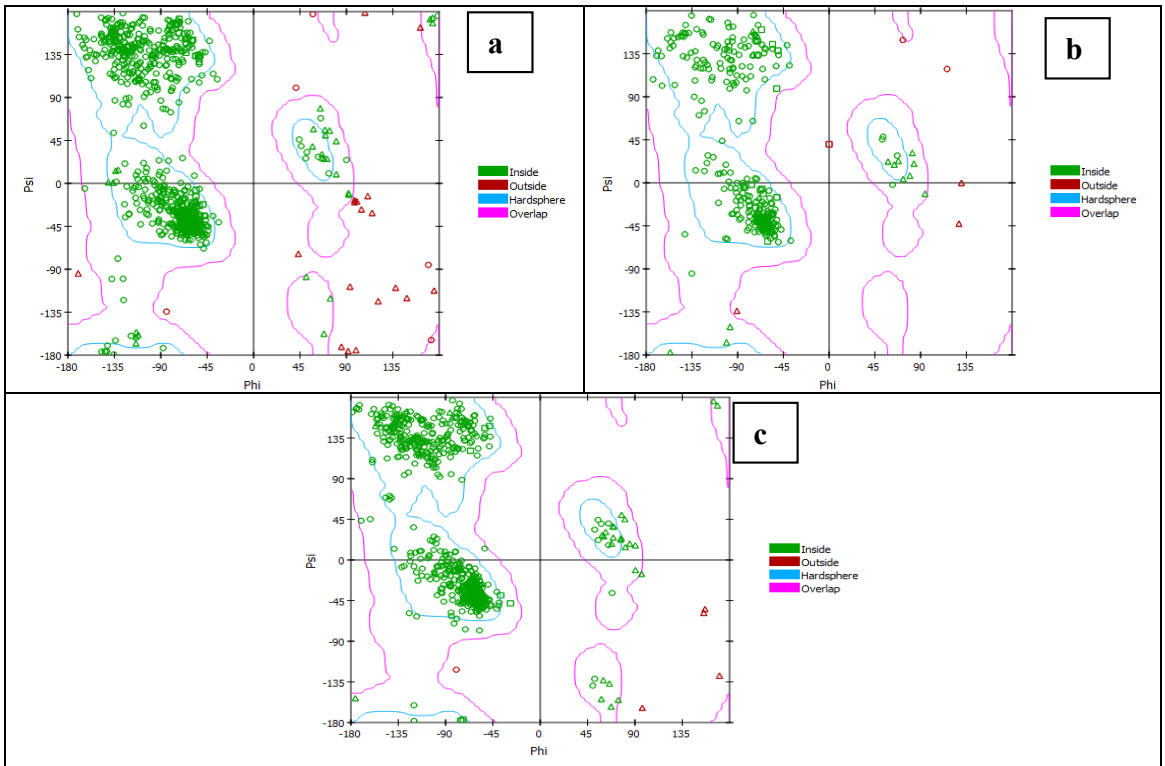
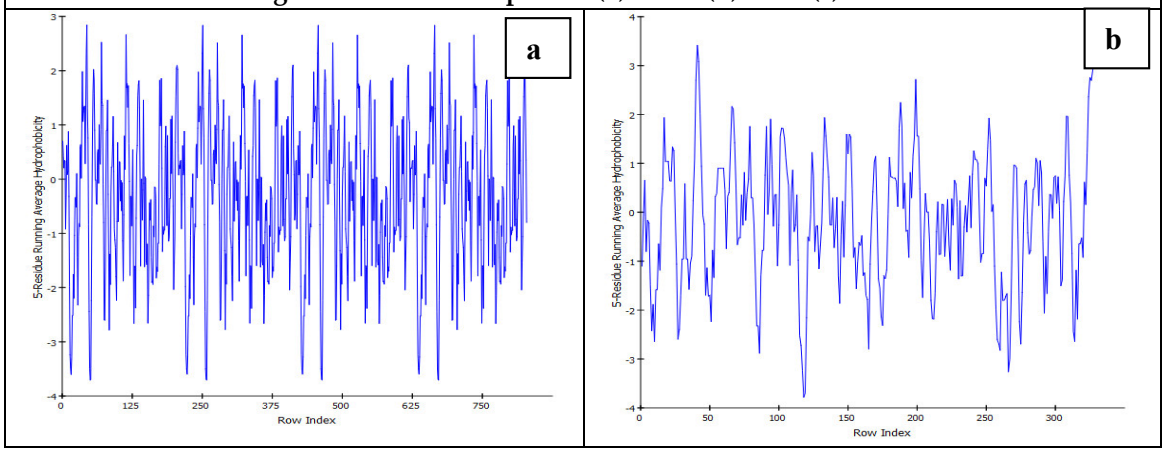


Fig 1: Ramachandran plot of (a) 3IWZ (b) 6B2S (c) 3KZC



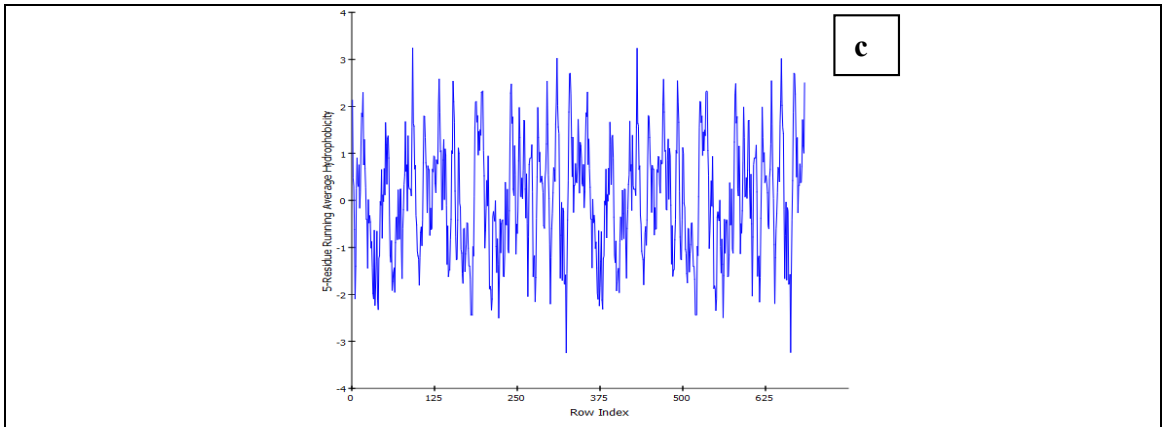


Fig 2: Hydrophobicity Plot of (a) 3IWZ (b) 6B2S (c) 3KZC

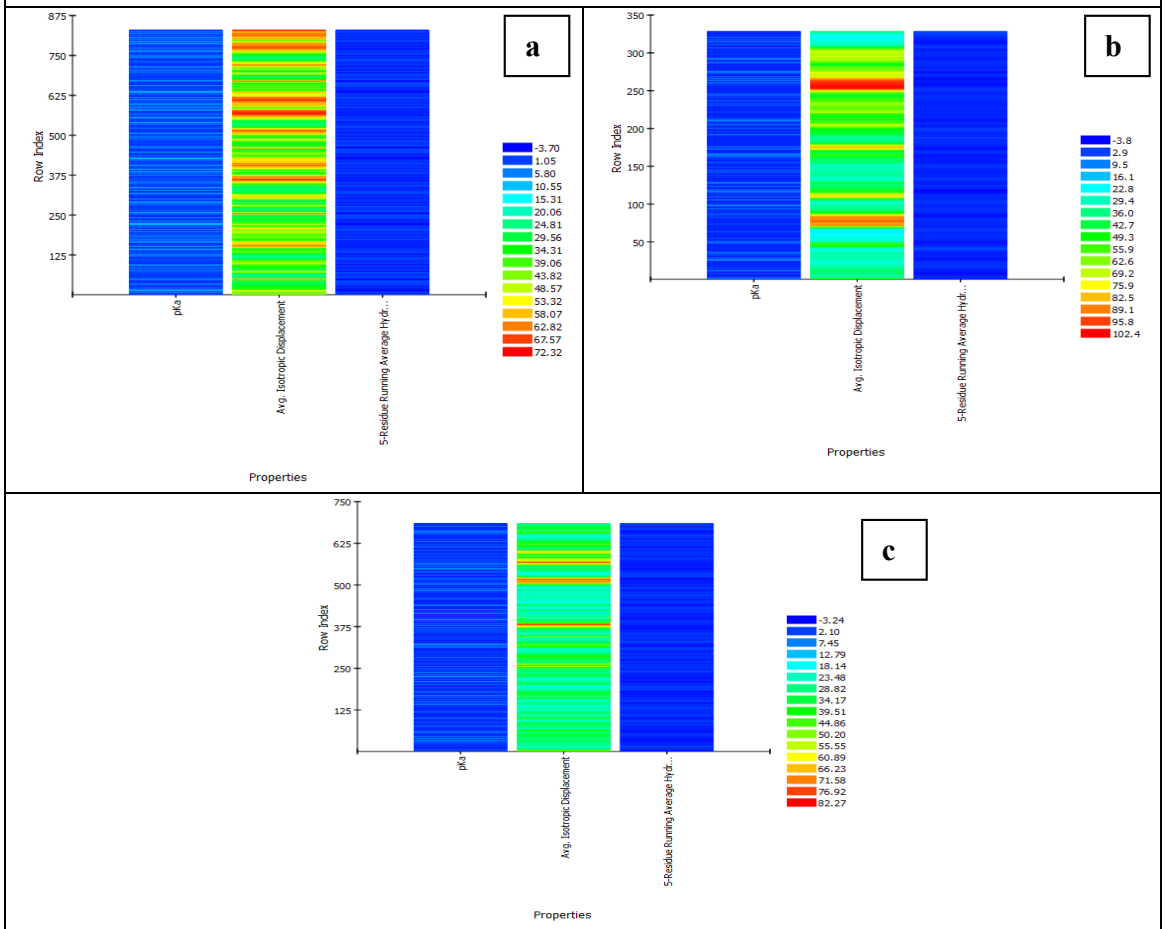


Fig 3: Heatmap Plot of (a) 3IWZ (b) 6B2S (c) 3KZC

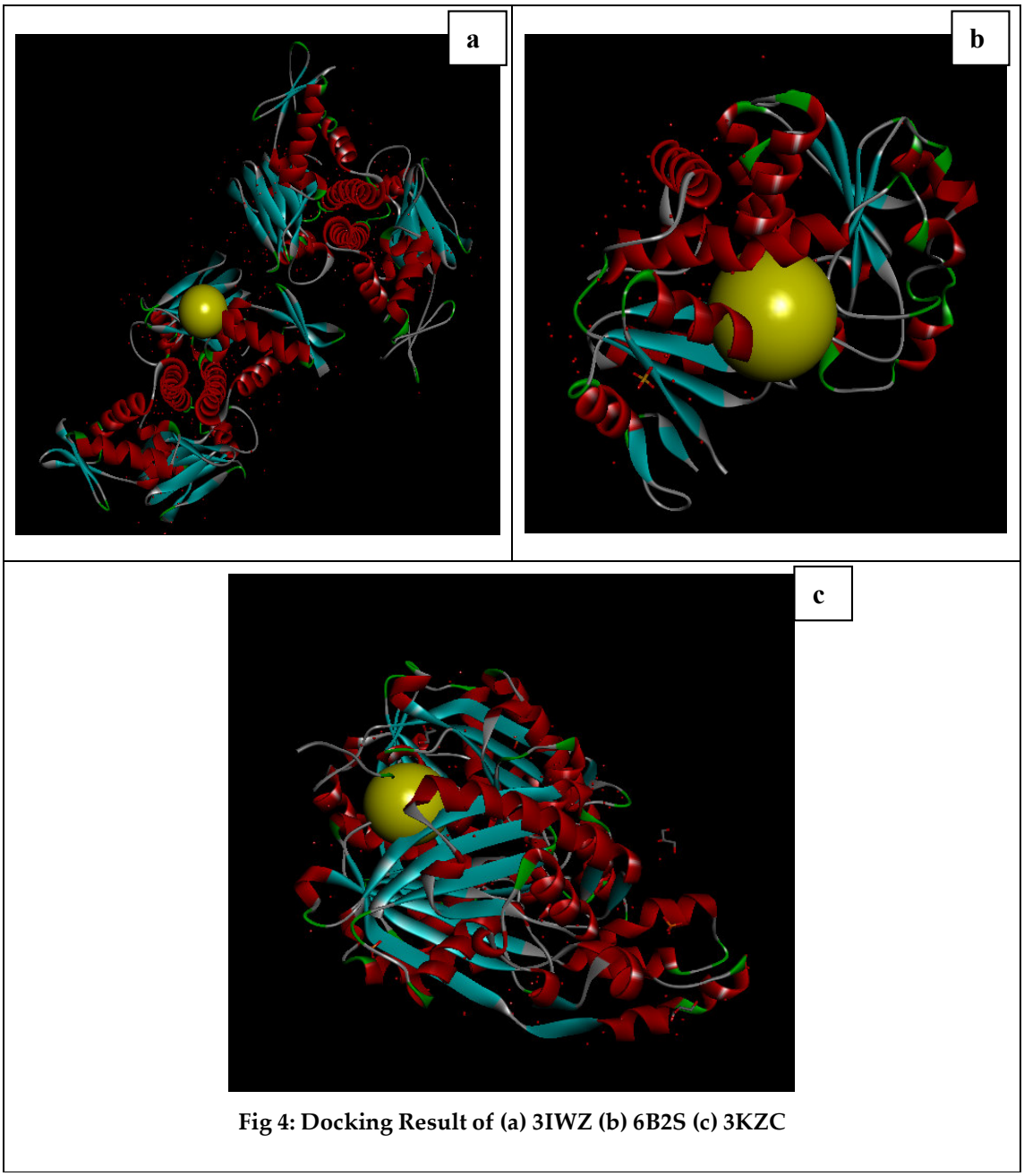


Fig 4: Docking Result of (a) 3IWZ (b) 6B2S (c) 3KZC

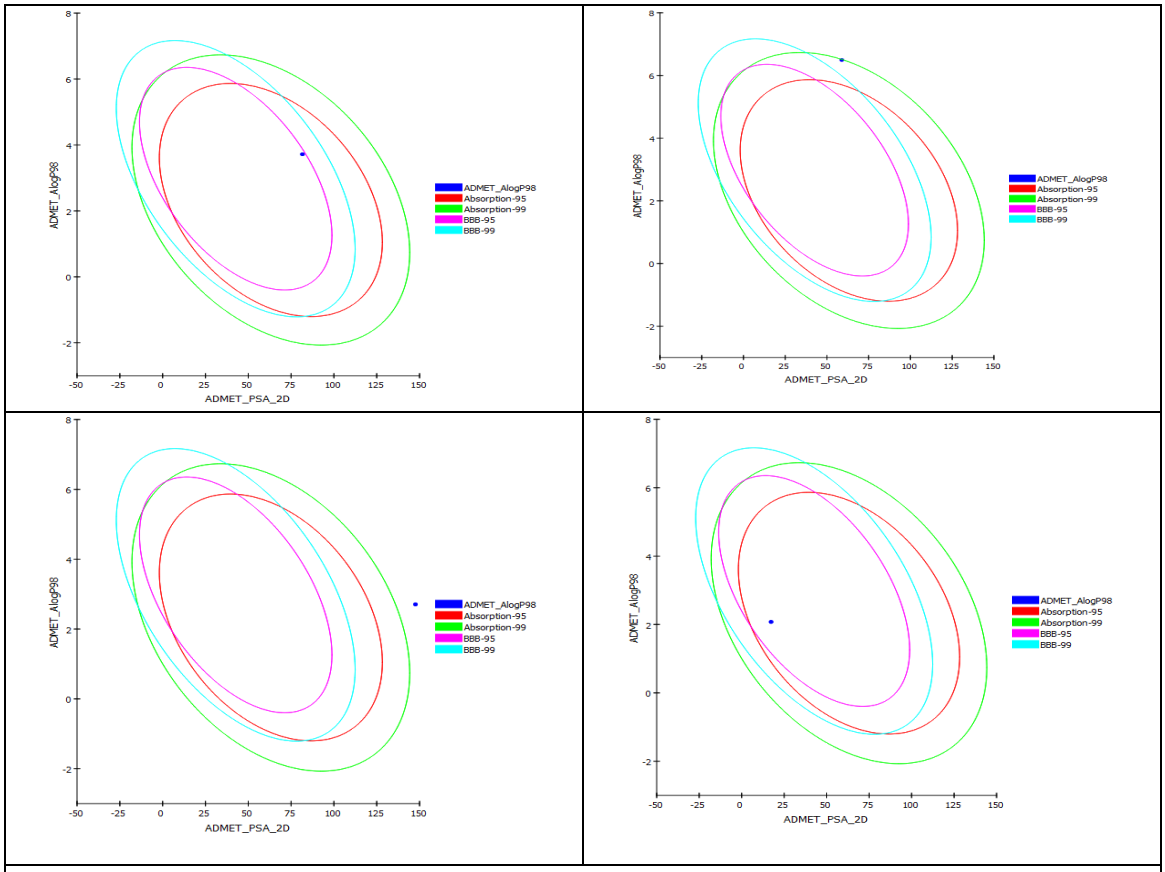


Fig 5: ADMET analysis Report

Table 1: The list of pharmacophores and the targeted genes from Black gram and green gram

Sl.No	Pharmacophores from Rosemary	Targeted Plant Disease Causing Microbial (Disease of black gram and green gram) Gene	PDB No of the Genes
1	Rosemerinic acid	cAMP-activated global transcriptional regulator CRP	3IWZ
2	Ursolic acid	3-oxoacyl-ACP synthase III	6B2S
3	Camphor	N-acetylornithine carbamoyltransferase	3KZC
4	Rosmadial		

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RESEARCH ARTICLE

In silico Analysis of the Green Chiretta (*Andrographis paniculata)* as Targeted Therapy for Targeted Plant Disease Causing Microbial Disease Chocolate Spot

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ABSTRACT

As aboriginal sources of medications, medicinal plants are used from the ancient times. *Andrographis paniculata* is one of the highly used potential medicinal plants in the world. This plant is traditionally used for the treatment of common cold, diarrhoea, fever due to several infective cause, jaundice, as a health tonic for the liver and cardiovascular health, and as an antioxidant. It is also used to improve sexual dysfunctions and serve as a contraceptive. All parts of this plant are used to extract the active phytochemicals, but the compositions of phytoconstituents widely differ from one part to another and with place, season, and time of harvest. We are using this property of Green Chiretta to get some new drugs for Chocolate Spot. The uses of various pesticides, preservatives, etc. turn the foods into poison. Moreover the side effects of these pesticides and preservatives, etc. are dangerous as because it leads to initiation of different cancer. In this whole world, the number of patients dying from cancer is increasing in a very threatening way. In-silico analysis has done using software and we further targeted some of the genes responsible for Chocolate Spot and pharmacophores from Green Chiretta and did some in silico analysis. In this we have found that these two pharmacophores are having better Mol Doc score from any others. From this we can deduce that these two pharmacophores can be a solution to pesticides in near future

Keywords: green chiretta, docking, in silico analysis, chocolate spot, pharmacophore

INTRODUCTION

Andrographis paniculata (Burm. F) Nees, commonly known as the "king of bitters," is an herbaceous plant belonging to the *A.canthaceae* and is found throughout tropical and subtropical Asia, Southeast Asia, and India. In India, *A.paniculata* is known as "Kalmegh"; in China it is known as "Chuan-Xin-Lian"; in Thailand it is known as "Fah Tha Lai"; in Malaysia it is known as "Hempedu bumi"; in Japan it is known as "Senshinren"; and in Scandinavian countries it is known as "green chiretta" (Chaudhary et. al, 2010). Extracts of this plant and andrographolide exhibit pharmacological activities such as those that are immunostimulatory (Joy et.al, 1998, Chaudhary et. Al, 2010), antiviral (Burkill et.al,1966), and antibacterial (Kavishankar et.al, 2011). As major active constituent, andrographolide exhibits a broad range of biological activities, such as anti-inflammatory, antibacterial, antitumor, antidiabetic, antimalarial, and hepatoprotective (Hajiaghaee and Akhondzadeh, 2012) Because of the impressive variety of these biological activities, researchers propose obtaining various leads by structurally modifying andrographolide. In recent decades, numerous andrographolide derivatives have emerged and their pharmacological activities have also been evaluated. However, studies that have comprehensively summarized or analyzed *A. paniculata* and its derivatives have been minimal. Therefore, to contribute to the advanced trends of research on andrographolide, this paper provides thorough information regarding the pharmacological activities of *A. paniculata* and its major compound andrographolide. Andrographolide is a major bioactive phytoconstituent found in various parts of *A. paniculata*, but particularly in the leaves. The chemical name of andrographolide is 3α, 14, 15, 18-tetrahydroxy-5β,9βH, 10α-labda-8, 12-dien-16-oic acid γ-lactone, and its molecular formula and weight are C20H30O5 and 350.4 (C 68.54%, H 8.63%, and O 22.83%), respectively. The structure of andrographolide has been analyzed by using X-ray, 1H,13 C-NMR, and ESI-MS (Jarukamjorn and Nemoto 2008, Akbar 2011, Kabir et.al. 2014, Urbi et al. 2014, Duke 2017). Although andrographolide is not very soluble in water, it is soluble in acetone, chloroform, ether, and hot ethanol. Crystalline andrographolide was reported to be highly stable, over a period of three months (Kumar et.al 2008). Some scientists reported a simple and rapid method for isolating andrographolide from the leaf of *A. paniculata*. Andrographolide has been reported to have a wide range of biological activities, such as those that are anti-inflammatory (Rajagopal et.al 2003), antiallergic (Cheung et al. 2005), antiplatelet aggregation (Liet al.v2007, Harjotaruno et.al 2008), hepatoprotective (Zhou et.al 2006).

MATERIALS AND METHODS

Phytochemicals of Ashwagandha have been listed with their structure data files which are taken from pubchem ChEBI. Genes has been taken randomly for Chocolate Spot using NCBI database. Table 1 has been showing the enlisted pharmacophores and the targeted genes. The PDB numbers of enzymes are taken from RCSB. The In-silico analysis has been done using BIOVIA –Discovery studio. We have performed various docking and used the Ramachandan plot and others.

Protein identification and preparation

The reported molecular targets responsible for Chocolate Spot are taken (Table 1) and the X-ray crystallographic structures of these target proteins were retrieved from protein data bank (PDB). The retrieved PDB structures contain water molecules, heavy atoms, cofactors, metal ions etc. and these structures do not have information about topologies, bond orders and formal atomic charges. Hence the downloaded PDB structures were prepared using 'prepare protein' protocol of Discovery Studio 4.0. The target proteins were prepared by removing all water molecules, ligands and other hetero atoms from the structures. Hydrogen atoms were added to the atoms to satisfy their valencies. The structures were then energy minimized by applying CHARM force field to remove the steric clashes between the atoms in order to get stable conformation.

Active site identification

The binding sites of the receptor proteins were predicted based on 'receptor cavity method' using Accelry's Discovery Studio 4.0. Using this protocol, active sites of the target receptor were identified based upon the inhibitory property of the amino acid residues present in the binding sites.

Ligand preparation and filtration

A collection of 5 phytocompounds from Green Chiretta were taken as ligands for docking analysis. The 3D structures of these compounds were downloaded from PubChem database. These ligands were then cleaned up, calculated 3D coordinates and generated ligand conformations by applying 'prepare ligand protocol' of Discovery Studio 4.0. After preparation, the compounds were filtered based on the molecular properties for predicting their solubility and permeability in drug discovery. The best known of the physical property filters is Lipinski's "rule-offive", which focuses on bioavailability. The rule states that the compounds have molecular mass less than 500 daltons, not more than 5 hydrogen bond donors, not more than 10 hydrogen bond acceptors and an octanol-water partition coefficient log P not greater than 5 **(Lipinski et al.,2001).** The filtered compounds were then used for docking analysis.

Docking

The anti-inflammatory activity of all the 4 phytochemicals reported from Green Chiretta was assessed by docking these compounds against the respective active sites of the target proteins. Discovery studio 4.0 was used in this study to find the interacting compounds of Green Chiretta with the selected targets of arthritis. Strategies of Discovery Studio 4.0 are to exhaustively dock or score possible positions of each ligand in the binding site of the proteins. Docking study of the target proteins was done with natural compounds derived from Green Chiretta to find the preferred orientation and binding affinity of the compounds with each target protein using scoring functions. A molecular dynamics (MD) simulated-annealing-based algorithm, namely, CDOCKER was used to score the interacting compounds. This method uses a gridbased representation of the protein-ligand potential interactions to calculate the binding affinity **(Wu et al., 2003).** CDOCKER uses soft-core potentials, which are found to be effective in the generation of several random conformations of small organics and macromolecules inside the active site of the target protein. Ligands were docked to the proteins followed by scoring them for their relative strength of interaction to identify candidates for drug development. The final poses were then scored based on the total docking energy, which is composed of intramolecular energy of ligand and the ligand-protein interaction. The lowest energy structure was taken as the best fit. Interpretation of the values was done using standards provided by Discovery Studio such as CDOCKER energy, CDOCKER interaction energy, hydrogen bonds, binding energy etc.

Drug likeliness

Drug-likeness is a qualitative concept used in drug design to evaluate how the substance acts like drug with respect to factors like bioavailability. The molecular properties which influence absorption, distribution, metabolism, excretion and toxicity are recognized as a long side therapeutic potency as key determinants of whether a molecule can be successfully developed as a drug **(Zhang et al., 2012).** These parameters are responsible for about 60 percent failures of all drugs in the clinical phases and so the prediction of ADMET properties plays a significant role in new drug discovery process (**Hire et al., 2012)**. Thus, it has become imperative to design lead compounds which would be easily Breast ly absorbed, easily transported to their targeted site of action, not easily converted into toxic metabolic products and easily eliminated from the body before accumulating in sufficient amounts. The ADMET properties of the compounds were analyzed for drug like candidates.

RESULT AND DISCUSSION

Protein preparation and active site identification

The three dimensional structures of the identified target proteins were retrieved from the protein data bank. PDB ID of the targeted protein structure are mentioned in Table 1.

Ramachandran Plot of the targeted gene

The Ramachandran plot is among the most central concepts in structural biology, seen in publications and textbooks alike. However, with the increasing numbers of known proteinstructures and greater accuracy of ultra-high resolution protein structures, we are still learning more about the basic principles of protein structure. The use of torsion angles to describe polypeptide and protein conformation was developed by Sasisekharan as part of his studies of the structure of collagen chains during his work as a graduate student in the research group of G.N. Ramachandran. The power of this approach was readily apparent and its use quickly became widespread. Using revised definitions, this so-called Ramachandran plot or φ, ψ-plot has remained nearly unchanged in the ensuing fifty years and continues to be an integral tool for protein structure research and education.

Hydrophobicity Plot of the Genes:

Protein–protein interactions (protein functionalities) are mediated by water, which compacts individual proteins and promotes close and temporarily stable large-area protein–protein interfaces. In their classic article, Kyte and Doolittle (KD) concluded that the "simplicity and graphic nature of hydrophobicity scales make them very useful tools for the evaluation of protein structures." In practice, however, attempts to develop hydrophobicity scales (for example, compatible with classical force fields (CFF) in calculating the energetics of protein folding) have encountered many difficulties.

Ligand preparation

4 of the pharmacophores are satisfied Lipinski rule and are expected to be active compounds after Breast administration. The ligand molecules with least binding energy are considered as compounds with highest binding affinity. This binding affinity indicated a focused interaction between the above compounds with the targets compared to others. The parameters for finding the best inhibitors such as CDOCKER energy, CDOCKER interaction energy and number of hydrogen bonds were also evaluated. CDOCKER energy is the combined energy produced by the sum of internal ligand strain energy and receptor-ligand interaction energy where, CDOCKER interaction energy is the interaction energy between the protein and ligand and the values of these two parameters indicate the strength of interaction between the proteins and the ligands. Besides least binding energy, compounds with least atomic energy difference between CDOCKER energy and CDOCKER interaction energy were analyzed. Based on CDOCKER energy and CDOCKER interaction energy, Fig 4 is showing the result.

CONCLUSION

The identified pharmacophores can be isolated from the Green Chiretta and can be commercialized as the natural drug for the Chocolate Spot which is having lesser harmful side effect from the chemotherapeutic drug available in the market. This drug will also be very cheaper from the available drugs and these drugs are also not harmful for the normal cells as they are derived from the natural products. The unique feature of the study is to targeted gene therapy for biopesticides. This will help our future medicine to be completely allied to the Pharmachophores and the uses of synthetic and carcinogenic drug will reduce.

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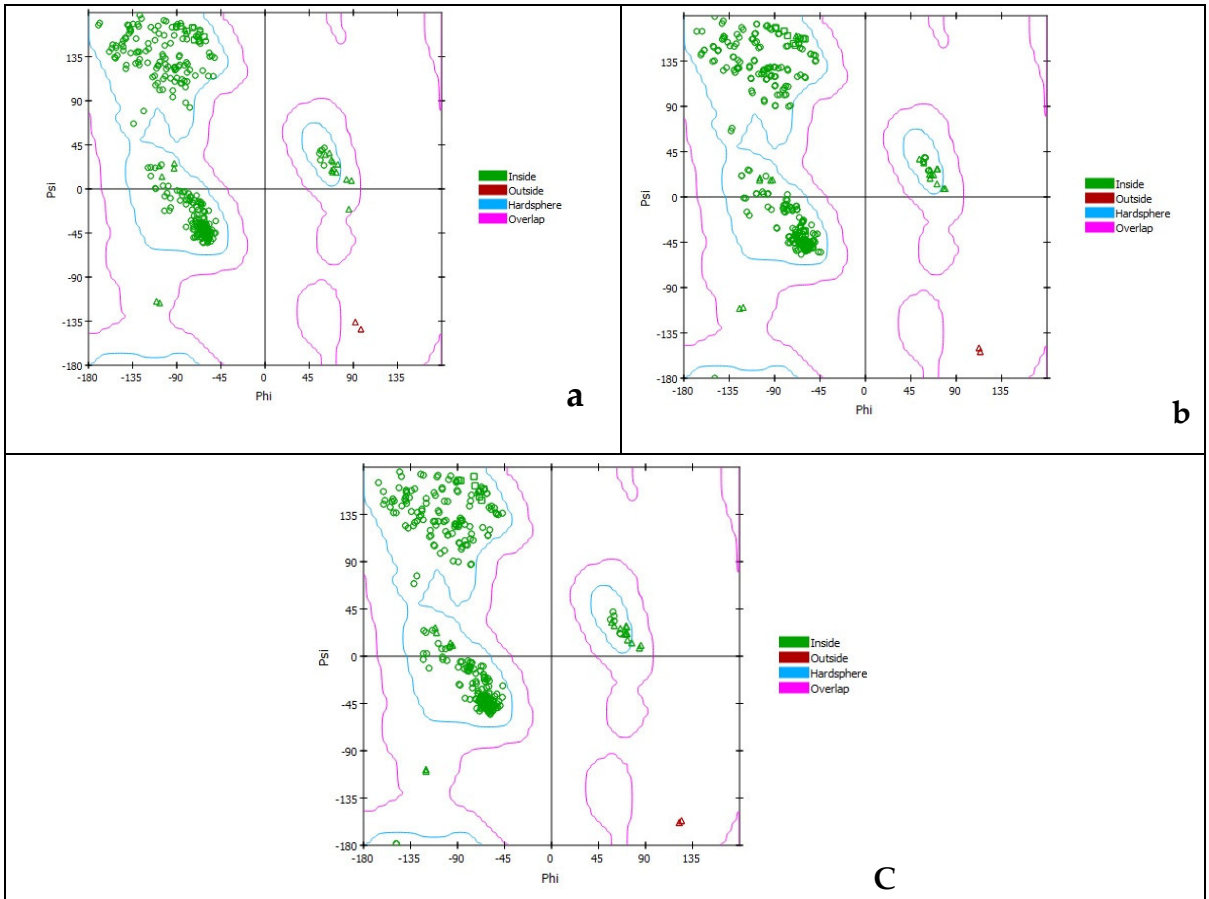
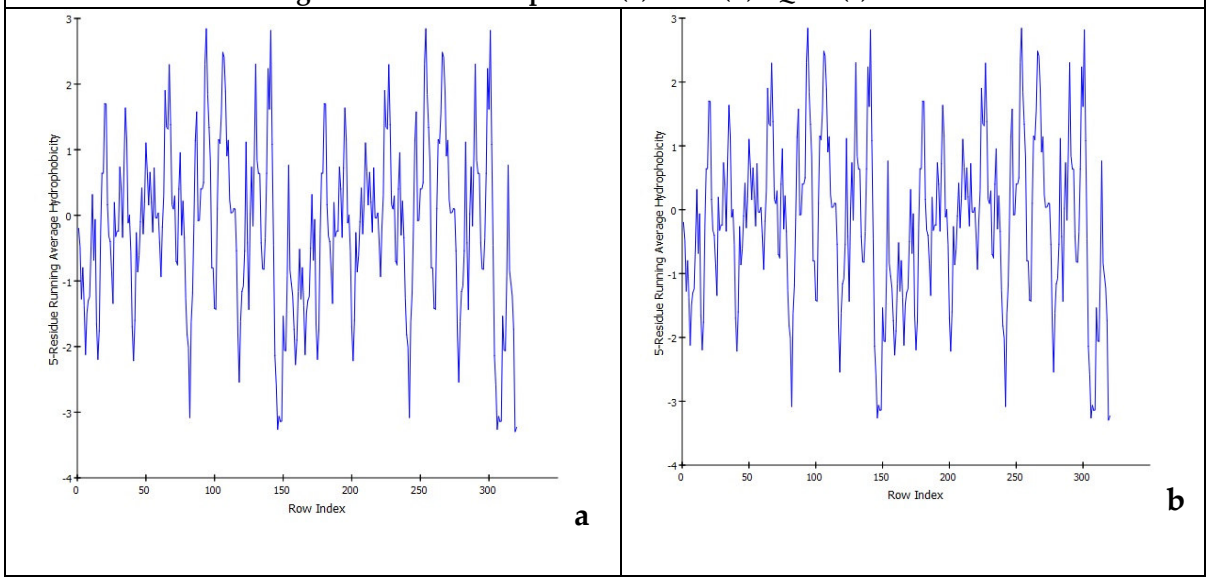


Fig 1: Ramachandran plot of (a) 6R0F (b) 6QZU (c) 6R0P



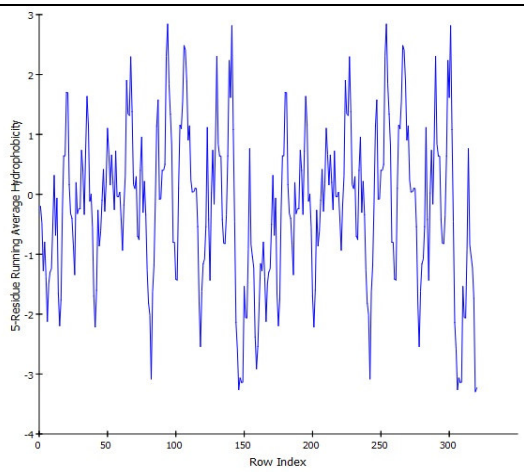


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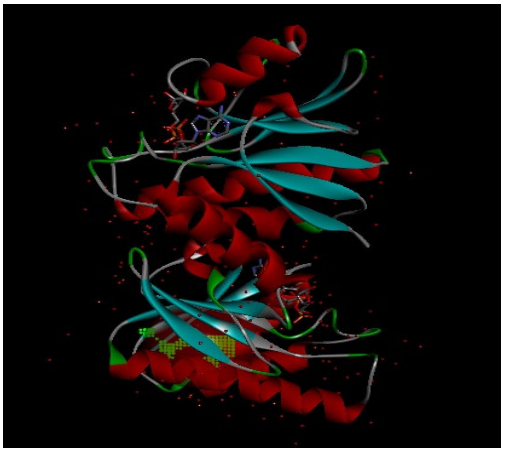
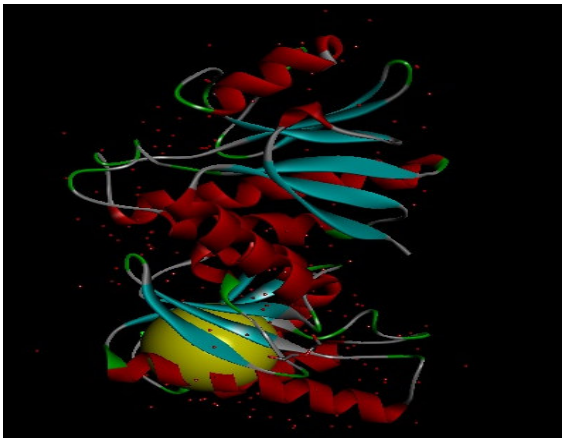
Fig 2: Hydrophobicity Plot of (a) 6R0F (b) 6QZU (c) 6R0P



a



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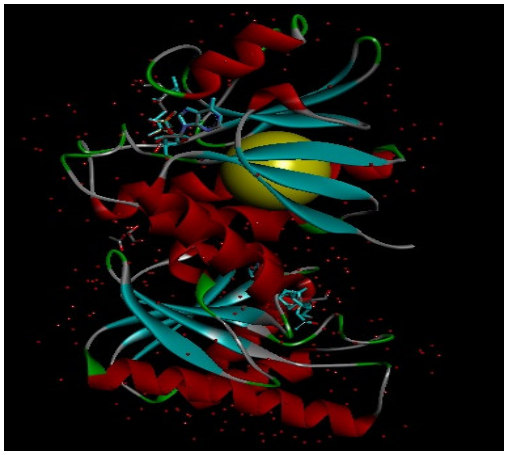

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Fig 3: Docking Result of (a) 6R0F (b) 6QZU (c) 6R0P

Table 1: The list of pharmacophores and the targeted genes from Chocolate Spot

Sl.No	Pharmacophores from Green Chiretta	Targeted Plant Disease Causing Microbial (Chocolate Spot) *Botrytis Cinera* Gene	PDB No of the Genes
1	Andrographolide	Tochv_S2_Gp2	6r0f
2	Neoandrographolide	Tochv_S2_Gp1	6qzu
3	14-Deoxy-11,12-Didehydroandrographolide	Tochv_S2_Gp1	6r0p
4	5,7,2′,3′-Tetramethoxyflavanone		

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REVIEW ARTICLE

A Review on Chemical Constituents and Pharmacological Studies of *Coriandrum sativum* L.

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ABSTRACT

Coriander (*Coriandrum sativum L.)* being a yearly herb is most generally utilized for flavoring reason. Its plant seeds, leaves and roots are palatable, in spite of the fact that they have unmistakable flavors and uses .It is an exceptionally mainstream restorative plant that has a place with Apiaceae family. The herb has a light and new flavor. Coriander can be utilized as entire plant and can be handled as a result of its transitory nature of leaves and to build the satisfactoriness of ready organic products (seeds) before utilizing it as seasoning operator in various food arrangements. Entire plant of coriander predominantly new leaves and ready organic products are utilized for culinary purposes. Coriander leaves have unexpected preference for comparison to its seeds, with citrus hints. Coriander plant is a rich store of micronutrients and dietary components which drives us to concentrate our investigation on this herb. Coriander is exceptionally low in soaked fat in any case, contains great measure of linoleic corrosive which is a decent wellspring of α-tocopherol and nutrient K. Leaves of plant are rich wellspring of nutrients while seeds are rich in polyphenols and basic oils. Coriander taste is given to its fundamental oil including a huge substance of linoleic and furanocoumarins (coriandrine and dihydrocoriandrine). Coriander is additionally notable for its cancer prevention agent, against diabetic, hostile to mutagenic, antianxiety and antimicrobial movement alongside pain relieving and hormone adjusting impact that advances its utilization in nourishments because of various medical advantages and its defensive impact to safeguard the nourishment for longer period.

Keywords: antioxidant content, anti-diabetic Coriandrum sativum, fatty acids,

INTRODUCTION

Coriander (*Coriandrum sativum L.*) which has a place with the family Apiaceae (Umbelliferae) is for the most part developed from its seeds consistently (Mhemdi et al., 2011). India is the greatest maker, shopper and exporter of coriander on the planet with a yearly creation of around three lakh tons. It is a yearly, herbaceous plant which started from the Mediterranean and Middle Eastern areas and known as therapeutic plants. The fundamental oils and concentrates of fragrant plants and flavors have been utilized in food conservation, pharmaceuticals, elective medication and normal treatments. As of now, it is important to research those plants logically, for the piece of basic oil (EO) and its natural exercises, which have been utilized in conventional medication to improve the nature of human services (Bhatta *et,al.,* 1989). The EO substance in various species are fluctuated characteristically, affected enormously by culture conditions and condition, just as by harvest and post-crop preparing, and henceforth assessments of the oils from numerous restorative plants are being directed. One of the most helpful EO bearing flavors just as therapeutic plants is *Coriandrum sativum L. (C. sativum)* (containing EO in its leaves, stem, blossoms and natural products/seeds) (Cerkauskas 2009).

South Asia is the world's greatest maker of coriander and a looming exporter to the nations like the USA, Middle East, EU, and South East Asia. World creation of coriander natural product is precarious to evaluate, since legitimate measurements inconsistently control figures identifying with this yield. An extensive greatness of coriander is developed in harping gardens or for a humble scope, and isn't recorded in any measurements. Enthralling the various explanations on this topic into account, the overall creation of coriander might be assessed at roughly 550,000 ha for each annum (Chakravarti and Rangrajan 1966).

CHEMICAL CONSTITUENTS

It incorporates: Monoterpene hydrocarbons viz α-pinene, β-pinene, limonene, γ-terpinene, ϱ-lymene, borneolXmphoe, Geraniol and Geranylacetate; Heterocyclic mixes viz – pyrazine, pyridine, thiazole, furan, tetrahydrofuran subsidiaries; Isocoumacin viz coriandrin, dihyrocoriandrin, coriandrones An E, glazonoids; Phthalides viz - neochidilide, Z-digustilide; Phenolic acids and sterols, flavonoids (Wallis, 2005). Carotenoids are of pervasive event in all plants with higher fixations in regenerative organs. In green verdant vegetables, carotenoids, especially β-carotene is kept basically in leaves. Carotenoids can likewise be prepared and utilized as shading specialists just as great wellspring of cancer prevention agents. Other than different jobs, carotenoids predominantly work as foragers of the free radicals created by chlorophylls during photograph oxidation. Its leaves being acceptable wellspring of β-carotene fill in as an antecedent of nutrient A. In coriander, β-carotene content, 160 μg/100 g is available though all out carotenoid content is 1010 μg/100 g (Kandlakunta et al., 2008). Its foliage is utilized in different sorts of nourishments particularly in diets of individuals confronting nutrient A lack. Green foliage contains anthocyanin (Omidbaigi, 2005). Anthocyanins are bioactive flavonoid intensifies that keep body from different ceaseless sicknesses. Anthocyanin in foliage goes about as cancer prevention agents which are extremely helpful in progress of dietary benefit just as upkeep of wellbeing (Chupp 1953). A scope of aldehyde mixes are to a great extent liable for the fragrance of coriander leaves. The biggest extent of these is those aldehydes with 6-10 carbon molecules, especially decyl (10) and nonyl (9) aldehydes. Other significant constituents of the leaves are 2-decenoic corrosive, decanoic corrosive (otherwise called capric corrosive) and tetradecenoic corrosive (Champawat, and Singh 2009).

PHARMACOLOGICAL EFFECTS

Antidiabetic effect

Organization of coriander seeds (5g/day) to NIDDM patients for 60 days essentially diminished lipid peroxidation, protein oxidation, diminished action of erythrocyte catalase (CAT), expanded serum β carotene, nutrient An, E and C in NIDDM diabetics. The treatment was additionally expanded the action of erythrocyte cell reinforcement compound for example glutathione-S-transferase (GST) and decreased glutathione content (GSH) in the rewarded

diabetics. The hypoglycemic impact of *Coriandrum sativum* was concentrated clinically in patients with type-2 diabetes mellitus. In the wake of measuring fasting plasma and urinary glucose, 10 patients of type-2 diabetes mellitus with no past medicine, 10 patients of type-2 diabetes mellitus taking oral hypoglycemic specialists with history of deficient control and six control subjects were given low (2.5 g tid) and high (4.5 g tid) dosages of watery and alcoholic concentrates of *Coriandrum sativum* for 14 days. On fifteenth day, blood and pee tests were taken for glucose estimation. *Coriandrum sativum* has huge hypoglycemic action in high portion and can be effectively joined with oral hypoglycemic operators in type-2 diabetic patients whose diabetes was not constrained by oral hypoglycemic medication alone. The hypoglycemic action of methanolic concentrates of leaves of *Coriandrum sativum* was assessed in rodents. The methanolic remove demonstrated critical portion dependant reduction in blood glucose level at a portion of 200 and 400 mg/kg. It likewise diminished the lipid parameters, for example, complete cholesterol, LDL, HDL, VLDL and TG when contrasted and diabetic control. SGOT and SGPT were diminished portion conditionally. Coriander fused into the eating routine (62.5 g/kg) and drinking water (2.5 g/l, arranged by 15 min decoction) decreased hyperglycaemia of streptozotocin-diabetic mice. A watery concentrate of coriander (1 mg/ml) expanded 2-deoxyglucose transport (1.6-overlap), glucose oxidation (1.4-overlay) and joining of glucose into glycogen of segregated murine muscular strength (1.7-crease) tantamount with 10-8 M-insulin. In intense 20 min tests, 0.25-10 mg/ml fluid concentrate of coriander evoked a stepwise 1.3-5.7-crease incitement of insulin emission from a clonal B-cell line. This impact was annulled by 0.5 mM-diazoxide. The impact of concentrate was potentiated by 16.7 mM-glucose and 10 mM-L-alanine however not by 1 mM-3-isobutyl-1-methylxanthine. Insulin discharge by hyperpolarized B-cells (16.7 mM-glucose, 25 mM-KCl) was additionally upgraded by the nearness of concentrate. Movement of the concentrate was seen as warmth stable, CH3)2CO solvent and unaltered by overnight introduction to corrosive (0.1 M-HCl) or dialysis to expel parts with atomic mass<2000 Da. Movement was decreased by for the time being introduction to soluble base (0.1 M-NaOH). Consecutive extraction with solvents uncovered insulin-discharging action in hexane and water portions showing a potential combined impact of more than one concentrate constituent. *Coriandrum sativum* (CS) supplementation (1% and 3% w/w) to high fat eating routine (HFD) mice (for 12 weeks) altogether forestalled HFD incited increase in body weight gain, food consumption, feed effectiveness, fasting blood glucose, plasma insulin, fasting insulin opposition record (FIRI), plasma and hepatic triglyceride (TG), all out cholesterol (TC), plasma free unsaturated fat (FFA), adipocyte width and surface region alongside decrement in adipocyte number. These arrangement of changes were similar to the rosiglitazone (0.05%) enhanced HFD took care of mice. The ethanol concentrate of *Coriandrum sativum* seeds was examined for its impacts on insulin discharge from the pancreatic beta cells in streptozotocin-prompted diabetic rodents. Pancreatic areas of 5 microm were handled for assessment of insulin-discharging action utilizing an immune cytochemistry technique. The outcomes demonstrated that organization of the ethanol extricate (200 and 250 mg/kg, ip) showed a noteworthy decrease in serum glucose. Then again, organization of streptozotocin diminished the quantity of beta cells with insulin secretory action in examination with flawless rodents, yet treatment with the coriander seed separate (200 mg/kg) expanded altogether the action of the beta cells in correlation with the diabetic control rodents. The potential hypoglycemic action of *Coriandrum sativum* (CS)- separate was examined after a solitary oral portion and after every day dosing for 30 days (sub-ceaseless investigation) in typical and large hyperglycemic-hyperlipidemic (OHH) rodents. A solitary portion of CS-concentrate or GLB stifled hyperglycemia in OHH rodents, and normoglycemia was accomplished at 6h post portion; there was no impact on lipids, TG or insulin, yet insulin opposition (IR) diminished fundamentally. The hypoglycemic impact was lower in typical rodents. In the subchronic concentrate in OHH rodents, the impact of (CS-extract> glibenclamide) with respect to diminishing plasma glucose (causing normoglycemia on day 21), expanding insulin and diminishing IR, TC, LDL-cholesterol, and TG. Atherosclerotic file was diminished, while cardioprotective files were expanded by CS-separate, with no impact on body weight, urea or creatinine. The antihyperglycaemic properties of the watery concentrate from the leaves and stems of Coriandrum sativum were assessed in normoglycaemic rodents, and on α-glucosidase action from Saccharomyces cerevisiae. Rodents were managed with the fluid concentrate of the plant at 100, 300 and 500 mg/kg, to watch the impact on oral sucrose resilience test. The fluid concentrate displayed noteworthy antihyperglycaemic movement at the three tried dosages. In vitro explores different avenues regarding α-glucosidase showed a serious kind hindrance. The antidiabetic and cancer prevention agent impacts of *Coriandrum sativum* (CS) were concentrated in alloxan-actuated diabetic rodents. The concentrates of

CS in alloxan-instigated diabetic rodents were found to essentially bring down blood glucose levels. Antidiabetic action of the CS extricates was tantamount with the clinically accessible medication glibenclamide. The degrees of serum complete cholesterol, triglycerides, and low-thickness lipoprotein cholesterol were lower in the extracttreated gathering and high-thickness lipoprotein cholesterol was higher than the diabetic control rodents. The concentrates of CS displayed solid rummaging impact on 2, 2-diphenyl-2-picrylhydrazyl free radical and restrained lipid peroxidation. The free radical rummaging impact of the concentrates was similar with that of the reference cancer prevention agents. Moreover, it additionally indicated an improved cancer prevention agent potential as confirm by diminished lipid peroxidation and a huge increment in the movement of different cell reinforcement proteins, for example, catalase, superoxide dismutase, and glutathione peroxidase in the liver of diabetic rodents (Singh 1946).

Anticancer effect

Salt water shrimp lethality bioassay uncovered that coriander LC50 was 2.25 mg/ml. The anticancer exercises of *Coriandrum sativum* root, leaf and stem, just as its impact on malignant growth cell relocation, and its assurance against DNA harm, with unique spotlight on the roots was assessed. The ethyl acetic acid derivation concentrate of *Coriandrum sativum* roots demonstrated the most noteworthy anti-proliferative action on MCF-7 cells (IC50 = 200.0 ± 2.6 µg/ml), had the most elevated phenolic substance and FRAP and DPPH searching exercises among the concentrates. Ethyl acetic acid derivation concentrate of *Coriandrum sativum* root restrained DNA harm and forestalled MCF-7 cell relocation instigated by H2O2, recommending its potential in malignant growth counteraction and metastasis hindrance. The concentrate showed anticancer movement in MCF-7 cells by influencing cancer prevention agent proteins potentially prompting H2O2 gathering, cell cycle capture at the G2/M stage and apoptotic cell passing by the demise receptor and mitochondrial apoptotic pathways. The antitumor and immune modulating exercises of watery and methanol concentrates of *Coriandrum sativum* (leaf and seed) was examined in vitro. The fluid concentrate of *Coriandrum sativum* (leaf), caused huge ($P<0.05$) 24, 39 percent L5178Y-R lymphoma cells harmfulness at 31.2 µg/ml (MIC), though the methanol concentrate of Coriandrum sativum (seed and leaf) caused 40 and 31 percent cytotoxicity at 7.8, 62.5 µg/ml (MICs), espectively. Furthermore, *Coriandrum sativum* leaf watery concentrate invigorated noteworthy ($P<0.01$) 14 to 45 percent splenic cells lympho proliferation at 7.8 to 125 µg/ml separately. The methanol concentrates of *Coriandrum sativum* leaf extricate caused huge ($P<0.01$) 43 to 59 percent lympho proliferation at the tried focuses. Besides, *Coriandrum sativum* watery concentrates were altogether ($P<0.01$) decrease up to 100% nitric oxide creation by LPS-animated macrophages. Three distinctive cell lines BMK (kidney), KHOS-2405 (bone), and WRL-68 (liver) were utilized to decide cytotoxicity. Cells were treated with various *Coriandrum sativum* (Cilantro) fixations (0.125%, 0.25%, 0.5%, 1%, 1.5%, 2% and 2.5%), for 24 hours. After this time, cytotoxic examinations were performed. An embryotoxicity study was finished utilizing prolific chicken eggs (gallus) vaccinating with *Coriandrum sativum* focuses (0.125%, 0.25%, 0.5%, 1%, 1.5%, 2% and 2.5%); hatched for 48 hours and watch them utilizing an electronic magnifying instrument to check the impacts. The three lines demonstrated diminished multiplication and number of cells corresponding to the focuses. The cell cycle examination indicated that *Coriandrum sativum* captured the WRL-68 cells in the (S) stage; the BMK cells were captured in the G2 and M stage, and the KHOS cells in the G1 stage. *Coriandrum sativum* delivered significant morphologic consequences for chicken incipient organisms. The utilization of *Coriandrum sativum* produces toxicological impacts on the incipient organisms just in high portions.

Cardiovascular effects

Coriander unrefined concentrate (1-30 mg/ml) caused fall in blood vessel pulse of anesthetized creatures which incompletely obstructed by atropine. Coriander unrefined concentrate delivered vasodilatation against phenylephrine and K+ (80 mM)- incited withdrawals in hare aorta and caused cardio-depressant impact in guinea-pig atria. Bioassay directed fractionation uncovered the partition of spasmogenic and spasmolytic segments in the fluid and natural divisions separately. Moreover, Coriander rough concentrate created diuresis in rodents at 1-10mg/kg. Fluid concentrates of coriander seeds hindered the electrically-evoked constrictions of winding strips and

rounded sections of disconnected focal ear supply route of hare (Harsha and Anilakumar 2016). The water concentrate of coriander seed had hypotensive impacts in rodents. The preventive impact of *Coriandrum sativum* (CS) on heart harm was assessed by isoproterenol instigated cardiotoxicity model in male rodents. Rodents were pretreated with methanolic concentrate of CS seeds at a portion of 100, 200 or 300 mg/kg orally for 30 days and they were hence regulated (sc) with isoproterenol (85 mg/kg body weight) throughout the previous two days. Isoproterenol rewarded rodents indicated expanded LPO, diminished degrees of endogenous cancer prevention agents and ATPases in the cardiovascular tissue along with expanded plasma lipids and markers of heart harm. TTC recoloring demonstrated expanded infarct regions while HXE recoloring indicated myofibrillar hypertrophy and interruption. CS (200 and 300 mg/kg body weight) pretreatment altogether forestalled or opposed every one of these changes. The outcomes indicated that methanolic concentrate of CS can forestall myocardial dead tissue by hindering myofibrillar harm. It is likewise proposed that, the rich polyphenolic substance of CS remove was answerable for forestalling oxidative harm by adequately searching the isoproterenol created ROS (Shivanand 2016).

CONCLUSION

Herbs and flavors are prepared in nourishments from early occasions for flavoring just as to expand timeframe of realistic usability of food and to reestablish wellbeing. Coriander is one of wonderful herb that capacities as both, zest just as home grown medication. In spite of the fact that plant can be developed consistently, it is handled to build its acceptability, gainfulness and encourage worldwide exchange. The leaves and organic products are exceptionally fragrant and contain supplements like fat, proteins, nutrients minerals and so forth. Its medical advantages exercises going from antibacterial to anticancer exercises. Generally significant and all around portrayed property of coriander is its utilization as cancer prevention agent. Because of its multifunctional utilizes and defensive and preventive activity against different constant sicknesses, this herb is righty called as "herb of bliss". Additionally, preparing of foods grown from the ground of coriander is the most ideal approach to save this herb. As indicated by the wide scope of pharmacological exercises, *Coriandrum sativum* ought to be considered as a promising wellspring of numerous medications as a result of its security and adequacy.

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RESEARCH ARTICLE

Amazon Sagemaker for Classifying Digital Images

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ABSTRACT

Image processing is a method to perform some operations on an image, in order to get an enhanced image or to extract some useful information from it. It is a type of signal processing in which input is an image and output may be image or characteristics/features associated with that image. The purpose of image processing is to improve the quality of the image by removing the disturbances. It consists of various techniques such as Image segmentation, enhancement, classification, restoration, pattern recognition, extraction etc. Image classification plays an important part in the fields of Remote sensing, Image analysis, Pattern recognition and many more. Digital image classification is the process of sorting all the pixels in an image into a finite number of individual classes. Here we discuss how Amazon SageMaker can be used for classification of digital images.

Keywords: Amazon SageMaker, Image Classification, Image Processing

INTRODUCTION

Digital imaging is a process to recognize objects of interest in an image by utilizing electronic devices and advanced computing techniques with the aim to improve image quality parameters. It contains basic difficulties due to the fact that image formation is basically a many-to-one-mapping. There are several problems associated with low-contrast images, blurred images, noisy images, image conversion to digital form, transmission, handling, manipulation, and storage of large-volume images, led to the development of efficient image processing and recognition algorithms. Digital imaging or computer vision involves image processing and pattern recognition techniques. Image processing techniques deal with image enhancement, segmentation, classification, restoration, reconstruction, manipulation and analysis of images etc. Digital image consists of discrete picture elements called pixels which are associated with a digital number represented as DN that depicts the average radiance of relatively small area with a scene. The range of DN values is normally 0 to 255. Digital Imaging advantages include:

- Accurate data acquisition
- Better combination of spatial and contrast resolution
- No degradation with time or copying
- Compact storage/easy retrieval
- Data correction/manipulation/enhancement
- Fast accurate image transmission

Classification of digital images generally comprises four steps

- Pre-processing. e.g. atmospheric correction, noise suppression, and finding the band ratio, principal component analysis, etc,
- Training: Selection of the particular feature which best describes the pattern,
- Decision: Choice of suitable method for comparing the image patterns with the target patterns
- Assessing the accuracy of the classification. The informational data are classified into supervised and unsupervised systems.

Image classification refers to the task of extracting information classes from a multi brand raster image. The resulting raster from image classification can be used to create thematic maps. Depending on the interaction between the analyst and the computer during classification, there are two types of classification: supervised and unsupervised.

Supervised classification

Supervised classification uses the spectral signatures obtained from training samples to classify an image. With the assistance of the Image Classification toolbar, you can easily create training samples to represent the classes you want to extract. We can also easily create a signature file from the training samples, which is then used by the multivariate classification tools to classify the image. In supervised classification, we select representative samples for each land cover class. The software then uses these "training sites" and applies them to the entire image. Supervised classification uses the spectral signature defined in the training set. For example, it determines each class on what it resembles most in the training set. The common supervised classification algorithms are maximum likelihood and minimum-distance classification.

Supervised Classification Steps

a) Select training areas
b) Generate signature file
c) Classify

Unsupervised classification

Unsupervised classification finds spectral classes (or clusters) in a multiband image without the analyst's intervention. The Image Classification toolbar aids in unsupervised classification by providing access to the tools to create the clusters, capability to analyze the quality of the clusters, and access to classification tools. In unsupervised classification, it first groups pixels into "clusters" based on their properties.

Unsupervised Classification Steps

a.Generate clusters
b.Assign classes

CLASSIFY IMAGES USING AMAZON SAGEMAKER

Amazon SageMaker is a fully managed service that supports all of the steps of a ML model's development: data exploration and building, training, and deploying ML models. With Amazon SageMaker, you can pick and use any of the built-in algorithms, reducing the time to market and the development cost. Traditional ML development is a complex, expensive, iterative process made even harder because there are no integrated tools for the entire machine learning workflow. You need to stitch together tools and workflows, which is time-consuming and error-prone. SageMaker solves this challenge by providing all of the components used for machine learning in a single toolset so models get to production faster with much less effort and at lower cost.

The Amazon SageMaker image classification algorithm is a supervised learning algorithm that supports multi-label classification. It takes an image as input and outputs one or more labels assigned to that image. It uses a convolutional neural network that can be trained from scratch or trained using transfer learning when a large number of training images are not available. The recommended input format for the Amazon SageMaker image classification algorithms is Apache MXNet RecordIO. However, you can also use raw images in .jpg or .png format.

The state-of-the-art technologies for image classification and object detection are based on deep learning (DL). DL is a subarea of machine learning (ML) that is focused on algorithms for handling neural networks (NN) with many layers, or deep neural networks. ML, in turn, is a subarea of artificial intelligence (AI), a computer-science discipline.

Understanding transfer learning

Transfer learning is a technique used for reducing the time required for training a new model. Instead of training your model from scratch, you can use a modified pre-trained model and continue training it with your dataset. That's why it's called transfer learning: the knowledge learned by one NN is transferring to another NN. It means, for instance, that if you want a model that can classify cars brand/model/year and you already have a pre-trained model, it makes sense to change it a little bit and retrain it with your own dataset in order to create a new model that will solve this new problem. The Amazon SageMaker built-in algorithm for image classification is already prepared for transfer learning. You just need to set a given parameter to true, and your model will use this technique.

Set up the environment

Make sure that the Role attached to your Jupyter Notebook Instance has the privileges for accessing S3. That instance will read and write to chosen S3 bucket. Now it's time to select the hyper parameters of your training environment. These parameters will determine how your model will be trained and, consequently, how your trained model will behave.

- **Num_layers:** the number of hidden/inner layers of your network. For small images chose a lower number, like [20, 32, 44, 56, 11].
- **Image_shape:** number of channels per width and height pixels of the images. That is, 3,28,28 where 3 is the number of color channels (RGB) and 28,28 are the width and height pixels of the images.
- **Num_classes:** number of classes that the model can classify
- **Mini_batch_size:** the number of images each batch will contain. Depending on how much VRAM your GPU has you can increase or decrease this size. A large size can cause an out-of-memory exception and the training will fail.
- **Epochs:** how many times the training algorithm will pass through your whole dataset. Depending on the algorithm you chose, each epoch will get only a random sample of your dataset for each epoch.

- **Learning_rate:** how fast the training algorithm will try to optimize your model. Lower learning rates can achieve best accuracy will take more time to train your model. Higher learning rates can fail to improve your model accuracy. You need to find a good balance for this attribute.
- **Use_pretrained_model:** if set to 1 it will enable Transfer Learning. Amazon SageMaker will get a pretrained Resnet with Imagenet 11K categories and customize it to your scenario.

After setting all these hyper parameters, you can select your instance, preferably a P2 or P3 instance with powerful GPUs, and start training your model.

Training the model

Amazon SageMaker is a platform based on Docker containers. Every built-in algorithm is a Docker image prepared with all of the libraries, frameworks, and binaries along with the algorithm itself. It turns the platform as flexible as possible. If you want to design your own ML algorithm, using your preferable technology just create a Docker image with your algorithm and call it from Amazon SageMaker. In this case, we will use an image that already contains the algorithm we need. This image will be used for creating a job that will train our model and then to publish the trained model in production as an endpoint. Depending on the region your Amazon SageMaker environment is running in, you'll need to select a different registry:

- us-west-2:dkr.ecr.us-west-2.amazonaws.com/image-classification:latest
- us-east-1:dkr.ecr.us-east-1.amazonaws.com/image-classification:latest
- us-east-2:dkr.ecr.us-east-2.amazonaws.com/image-classification:latest
- eu-west-1:dkr.ecr.eu-west-1.amazonaws.com/image-classification:latest

Next, you have to create a job description. The job description is a structure with all the parameters and hyper parameters you have set that will be sent to Amazon SageMaker so that SageMaker can then start a job for you. The result of this process is the trained model that will be saved to the S3 bucket you chose. You can monitor each step of the training process through CloudWatch Logs and Metrics, as shown in the following image. Just click in the running job in the Amazon SageMaker console and go to the Monitor session. If you want to see how much GPU memory is being utilized or what is the GPU or CPU utilization, just go to Amazon CloudWatch metrics.

Testing and deploying the model

The following steps are needed:

- Convert the job output in a model that will be available in the Amazon SageMaker model catalog.
- Create an endpoint configuration. In this step, you decide which instance will support your predictions. It is possible to train your model in a machine with GPU and then deploy it on a CPU only machine. That's what we'll do in our hands on. Deploying your model to a CPU only instance can reduce your costs.
- Deploy your model, using the endpoint configuration defined previously. Amazon SageMaker will create an instance for you and deploy a container with the algorithm you've selected. Inside that container, your trained model will be hosted. After that, you will be able to send requests to that endpoint by using an API.

CONCLUSION

Amazon SageMaker helps you create a powerful solution for your image-classification needs. You can focus on the creation process and the business problem itself while Amazon SageMaker gives you a flexible and elastic infrastructure for supporting your ML pipeline.

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Fig. 1. Details of Amazon SageMaker

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RESEARCH ARTICLE

Aws Iot Analytics to Analyze Forest Fire Images

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ABSTRACT

The most common hazard in forests is forests fire. They pose a threat not only to the forest wealth but also to the entire regime to fauna and flora seriously disturbing the bio-diversity and the ecology and environment of a region. A forest fire is a disaster and threat not only to the forest but also to the wild animals, the entire ecology and to the environment. The early detection and monitoring of forest fire with accuracy leads to a boon to the wild life and the inhabitants because, as soon as the detection and monitoring is processed, the necessary and quick actions to that can be taken in time. Here we are discussing how AWS IoT Analytics can be used to analyze forest fire so that effective and in-time action can be taken in an optimized way

Keywords: AWS IoT Analytics, Forest fire

INTRODUCTION

Forest plays an important role in the balancing of environment, socio-ecological and recreational system. [3] In India the total forest and tree cover is 79.42 million hectare, which is 24.16 % of the total geographical area. Forests have high impact in balancing the equilibrium in atmospheric carbon absorption, regulation of temperature and rainfall, reduction of soil erosion etc. Forest fire also known as Wildfire is a severe disaster [4] which has negative effect on socio- ecological and economical balances. Every year thousands hectares of forest territory is ravaged due to this forest fire. In 2016 more than 4000 hectares of forest were destroyed in the hills of Uttarakhand due to various reasons of forest fire. In some cases forest fire leads to the death of the inhabitants at the affected zone. The main cause of forest fire may be natural like lightning, rolling of stones, and rubbing of dry bamboos due to strong winds or may be accidental fires created due to human carelessness. Forest fire is considered to be one of the causes of global warming. Forest fire detection methods mainly consist of patrolling, observation from watch towers, satellite monitoring or harbour watch system.

The conventional methods like patrolling, watchtowers are easy but not effective. The problems with these methods are carelessness of guards, absence from the post, inability for real-time monitoring and the limited area coverage

etc. The satellite based monitoring is a popular and most widely used method [4][10] but it requires a long scan cycle and till the completion, fire may have spread in an uncontrolled way. This method covers broad areas but resolution of images is low [5] and sometime clouds and fogs may mask the images which lead to distorted image broadcasting. Forest Watch [11] is another forest fire detection system. These systems are operational in different countries like South Africa (83 towers), USA (22 towers), Swaziland (5 towers), Canada (4 towers), Chile (20 towers), and Slovakia (4 towers). The Harbour Watch system has been deployed in South Africa and Namibia [12] as shown in fig. 1. In this approach fire is reliably detected up to a range of 20 km but sometime it generates false alarms. So here we proposed the use of wire- less sensor network as a real-time, energy efficient model in detecting forest fire.

AWS IOT ANALYTICS

AWS IoT Analytics is a fully-managed service that makes it easy to run and operationalize sophisticated analytics on massive volumes of IoT data without having to worry about the cost and complexity typically required to build an IoT analytics platform. It is the easiest way to run analytics on IoT data and get insights to make better and more accurate decisions for IoT applications and machine learning use cases. IoT data is highly unstructured which makes it difficult to analyze with traditional analytics and business intelligence tools that are designed to process structured data. IoT data comes from devices that often record fairly noisy processes (such as temperature, motion, or sound). The data from these devices can frequently have significant gaps, corrupted messages, and false readings that must be cleaned up before analysis can occur. Also, IoT data is often only meaningful in the context of additional, third party data inputs. For example, to help farmers determine when to water their crops, vineyard irrigation systems often enrich moisture sensor data with rainfall data from the vineyard, allowing for more efficient water usage while maximizing harvest yield. AWS IoT Analytics automates each of the difficult steps that are required to analyze data from IoT devices. AWS IoT Analytics filters, transforms, and enriches IoT data before storing it in a time-series data store for analysis. You can setup the service to collect only the data you need from your devices, apply mathematical transforms to process the data, and enrich the data with device-specific metadata such as device type and location before storing the processed data. Then, you can analyze your data by running ad hoc or scheduled queries using the built-in SQL query engine, or perform more complex analytics and machine learning inference. AWS IoT Analytics makes it easy to get started with machine learning by including pre-built models for common IoT use cases. You can also use your own custom analysis, packaged in a container, to execute on AWS IoT Analytics. AWS IoT Analytics automates the execution of your custom analyses created in Jupyter Notebook or your own tools (such as Matlab, Octave, etc.) to be executed on your schedule.

AWS IoT Analytics benefits

- Operationalize your analytical workflows
- Easily run queries on IoT data
- Data storage optimized for IoT
- Prepares your IoT data for analysis
- Tools for machine learning

Automated scaling with pay as you go pricing.

HOW AWS IOT ANALYTICS WORKS

a) Collect

- Integrated with AWS IoT Core—AWS IoT Analytics is fully integrated with AWS IoT Core so it can receive messages from connected devices as they stream in.
- Use a batch API to add data from any source—AWS IoT Analytics can receive data from any source through HTTP. That means that any device or service that is connected to the internet can send data to AWS IoT Analytics.
- Collect only the data you want to store and analyze—You can use the AWS IoT Analytics console to configure AWS IoT Analytics to receive messages from devices through MQTT topic filters in various

formats and frequencies. AWS IoT Analytics validates that the data is within specific parameters you define and creates channels. Then, the service routes the channels to appropriate pipelines for message processing, transformation, and enrichment.

b) Process

- Cleanse and filter—AWS IoT Analytics lets you define AWS Lambda functions that are triggered when AWS IoT Analytics detects missing data, so you can run code to estimate and fill gaps. You can also define maximum and minimum filters and percentile thresholds to remove outliers in your data.
- Transform—AWS IoT Analytics can transform messages using mathematical or conditional logic you define, so that you can perform common calculations like Celsius into Fahrenheit conversion.
- Enrich—AWS IoT Analytics can enrich data with external data sources such as a weather forecast, and then route the data to the AWS IoT Analytics data store.

c) Store

- Time-series data store—AWS IoT Analytics stores the device data in an optimized time-series data store for faster retrieval and analysis. You can also manage access permissions, implement data retention policies and export your data to external access points.
- Store processed and raw data—AWS IoT Analytics stores the processed data and also automatically stores the raw ingested data so you can process it at a later time.

d) Analyze

- Run Ad-hoc SQL queries—AWS IoT Analytics provides a SQL query engine so you can run ad-hoc queries and get results quickly. The service enables you to use standard SQL queries to extract data from the data store to answer questions like the average distance traveled for a fleet of connected vehicles or how many doors in a smart building are locked after 7pm. These queries can be re-used even if connected devices, fleet size, and analytic requirements change.
- Time-series analysis—AWS IoT Analytics supports time-series analysis so you can analyze the performance of devices over time and understand how and where they are being used, continuously monitor device data to predict maintenance issues, and monitor sensors to predict and react to environmental conditions.
- Hosted notebooks for sophisticated analytics and machine learning—AWS IoT Analytics includes support for hosted notebooks in Jupyter Notebook for statistical analysis and machine learning. The service includes a set of notebook templates that contain AWS-authored machine learning models and visualizations. You can use the templates to get started with IoT use cases related to device failure profiling, forecasting events such as low usage that might signal the customer will abandon the product, or segmenting devices by customer usage levels (for example heavy users, weekend users) or device health. After you author a notebook, you can containerize and execute it on a schedule that you specify.
- Prediction—You can do statistical classification through a method called logistic regression. You can also use Long-Short-Term Memory (LSTM), which is a powerful neural network technique for predicting the output or state of a process that varies over time. The pre-built notebook templates also support the K-means clustering algorithm for device segmentation, which clusters your devices into cohorts of like devices. These templates are typically used to profile device health and device state such as HVAC units in a chocolate factory or wear and tear of blades on a wind turbine. Again, these notebook templates can be contained and executed on a schedule.

e) Build and visualize

- Amazon QuickSight integration—AWS IoT Analytics provides a connector to Amazon QuickSight so that you can visualize your data sets in a QuickSight dashboard.
- Console integration—You can also visualize the results or your ad-hoc analysis in the embedded Jupyter Notebook in the AWS IoT Analytics' console.

CONCLUSION

AWS IoT Analytics automates the steps required to analyze data from IoT devices. AWS IoT Analytics filters, transforms, and enriches IoT data before storing it in a time-series data store for analysis. You can set up the service to collect only the data you need from your devices, apply mathematical transforms to process the data, and enrich the data with device-specific metadata such as device type and location before storing it. Then, you can analyze your data by running queries using the built-in SQL query engine, or perform more complex analytics and machine learning inference. AWS IoT Analytics enables advanced data exploration. So this can be used to analyze forest fire data so that a quick, effective and in-time action can be taken.

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Fig. 1 Harbour watch system [12]

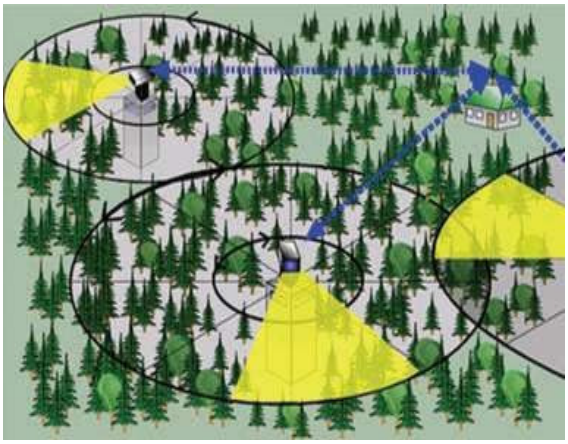

Fig. 2 Fire watch system [13]

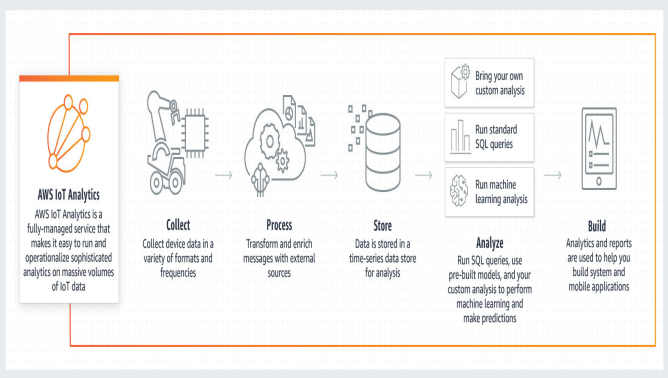

Fig.3. Aws iot analytics works

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RESEARCH ARTICLE

Design of a Flower Shaped Dipole Antenna

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ABSTRACT

A flower shaped patch over the substrate is proposed in this article. This antenna act as a dipole antenna.It consists of a substrate, a radiator, a ground and a port. When we give signal to the wave port the antenna works. This proposed antenna main a compact structure. The simulated ones, giving a wide impedance bandwidth of 1.68 to 2.75 GHz, a high port-to-port insulation (better than 37 dB) within the operating frequency bandwidth, and a good radiation pattern. In fact, the suggested antenna retains a compact configuration of 0.78 λ_0 × 0.78 λ_0 0.18λ_0. This antenna is designed for 2G/3G / LTE base station as this antenna is built with a compact framework so.

Keywords: Flower shaped patch, dipole antenna, polarization, return loss, radiation pattern.

INTRODUCTION

The base station antennas with broad impedance array, high port insulation secure radiation pattern, low cross polarization and low profile are in great demand due to the rapid growth of electronic communication. Dual-polarized antenna shares which are widely used in base stations for mobile communication to improve system performance by using diversity of polarization. In base stations, it became common and contributes to their successful success in reducing multi-path fading and growing channel power[1-2].

This consists of two such broadband antenna elements positioned orthogonally to one another for dual polarization operation.Various dual-polarized antennas have recently been suggested as base station antennas with variable structures such as patch antenna dipole antenna, crossed-dipole antenna, crossed-slot antenna and multi-dipole antenna. A patch antenna is a type of low-profile radio antenna which can be placed on a flat surface. This consists of a thin rectangular sheet of metal, placed on a wider sheet of metal called a ground plane [3-4]. Patch antennas are common because the advantages of low profile, low cost and ease of mass manufacturing. The shorted patch antenna or planer antenna is a version of the patch antenna widely found in cell phones [8-9].

One corner of the patch is grounded in this antenna, with a ground plate. Thanks to their low weight, capacity to adapt to any geometrical structure, and simple incorporation and low-cost manufacturing, the patch antennas are very useful. Their main drawback is their narrow bandwidth, unfit for wireless communication [6]. This can give

performance in bandwidth, and it can also reconfigure frequency. This article opens with brief introduction of basic features, feeding method, and patch antenna analysis techniques.Also, an option for dual polarization is a cross-shaped slot antenna excited by two orthogonal staggered microstrip feed sheets. As well as the stepped microstrip feed lines, stepped impedance slot and small crossed slot were also used to suit impedance over a large bandwidth [10].To achieve dual polarization and a high 40 dB isolation covering a wide bandwidth, a multi-dipole antenna is introduced in. Yet due to its crown-shaped structure, its manufacturing may be difficult.

Antenna parameters

Parameters of antennas are

a) Gain
b) Radiation pattern
c) Bandwidth
d) Polarization
e) Impedance.

The antenna pattern is the antenna 's response from a given direction to a plane wave incident, or the relative power density of the wave which the antenna transmits in a given direction.

Radiation pattern of the antenna

A radiation pattern defines the power variation which an antenna radiates as a function of the direction away from the antenna. This strength variance is observed as a function of the angle of arrival in the far field of the antenna.

Types of Radiation pattern

- Power pattern: -Trace of angular variation of the power received from antenna at a constant radius.
- Amplitude field pattern: -Analysis of the spatial variance in electric field amplitude at a constant antenna radius.

Directivity

Directivity is an essential parameter of antennas. It is a measure of how 'directional' the radiation pattern in an antenna is. An antenna that radiates in both directions similarly would have zero directionality and 1 (or 0 dB) would be the direction of this type of antenna.

DIPOLE ANTENNA

In this a dipolar antenna is introduced. The antenna consists of a radiator, a cross-shaped slot coupler, a pair of baluns with microstrips and a reflector. The cross-shaped slot coupler will act as a four-way equal-split power divider while baluns are excited and produce four differential signals at four ends of the slot lines. The signals would then be coupled to four modified dipoles in order to radiate and synthesize linear polarization in the slant ±45 °. The design proposed is verified through the manufacture and testing of a prototype antenna. The signals would then be coupled to four modified dipoles in order to radiate and synthesize linear polarization in the slant ±45 °.

Types of Dipoleantenna

Half wave dipole antenna

The most widely used half-wave dipole antenna is the one. It is a resonant antenna, being a half wavelength long. The dipole half-wave antenna is just a special case of the dipole antenna, but it’s important enough to have its own section. Note that the term "half-wave" means that at the operating frequency, the length of this dipole antenna is equal to one half-wavelength.

Folded dipole antenna

Because the name means this type of the aerial dipole or dipole antenna is folded back on itself. Although the gap between the ends of half a wavelength is always retained, an extra conductor gap essentially links the two ends together.

Short dipole

A short dipole antenna is one that is much less in duration than half a wavelength. Where a dipole antenna is shorter than half a wavelength, the impedance to feed starts to increase, and its response is less dependent on frequency changes.

Non-resonant dipole

A dipole antenna with a high impedance feeder and operate away from its resonant frequency. That allows it to work across a much broader bandwidth.

Broadband dipole antenna-By through the amount it occupies an antenna may be rendered broadband. Thus, by increasing the dipole's radius, a dipole antenna can become more broadband. Such antennas are also classified as dipole wideband.

Antenna Parameters

There are many criteria to consider when choosing an antenna for a wireless system. Two of the most significant aspects to consider include how the interference differs in the various ways across the antenna, how effective the antenna is, the frequency that the antenna provides the best output and the antenna that suits optimum power transmission.

DESIGN of FLOWER SHAPED ANTENNA

A reconfigurable antenna based was simulated for frequency polarization. Application of Rogers RO4003C substrate with a 3.55 dielectric constant and a 32 mm width. The configured antenna dimension is as shown in figure: W=1.72 mm, L=48.7 mm, T=0.8 mm. Figure 1 shows the flower shaped patch design over the substrate using HFSS.

SIMULATION RESULT

The proposed antenna simulation parameter with different angles of rotation is shown in the diagram. The test indicates that the antenna 's operational frequency spectrum does not differ with the rotation angle shift. It can be shown that the effects of the calculation are compatible with the outcome of the simulation. Consequently, the antenna 's working frequency varies from 7.3 to 11.5GHz. Both measured and simulated parameters are less than -10dB throughout the entire band width.

The operating frequency of both RHCP and LHCP operating modes may therefore be replicated by changing the angle between the slot antenna, the MS and the metallic reflector. The bandwidth of estimated 3dB is 3.2GHz.

The calculated and simulated radiation trend and the potential antenna gains at 8.5GHz are shown in the figure for specific radiation angel. The antenna pattern measurements are done only around the main beam to get more accurate test results. It can be seen that for slot antenna the antenna has directional radiation patterns rather than bidirectional radiation pattern. It's obvious that by decreasing the size, the bore sight gain is increased. The maximum gain measured, at 10.5 GHz, is 15.5dBi.

Radiation Pattern

The findings of the microstrip dipole antenna were explored with respect to bandwidth, characteristic radiation pattern and cross-polar isolation relative to monopoly antenna.

The return loss simulation result of flower shaped dipoleantenna is shown in figure 2.

CONCLUSION

A low-cost dipole microstrip antenna has been proposed for WLAN operations in the 2.4GHzband. The antenna proposed is small in diameter, which is simple to install. The antenna radiates bidirectional in the E-plane by having its dipole near one half wavelengths. The prototype was the dipole, and was tested. Microstrip dipole bandwidth is 14.68 per cent higher than mono pole antenna. The microstrip dipole antenna's cross-polar insulation is within the range of 3 to 17.32 dB. The full cross-polar insulation can be seen at H Plane. The HPBW for dipole microstrip is 60º for E plane and 75º for H plane.

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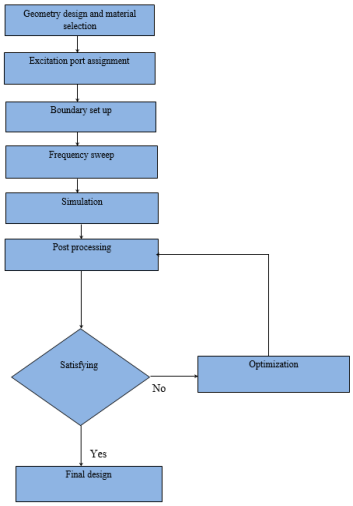

Figure 1. Flow chart of antenna design

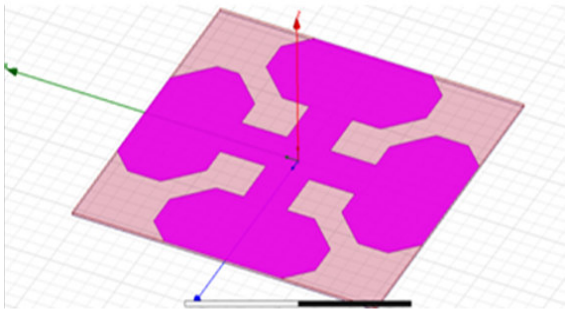

Figure 2. Antenna design using HFSS

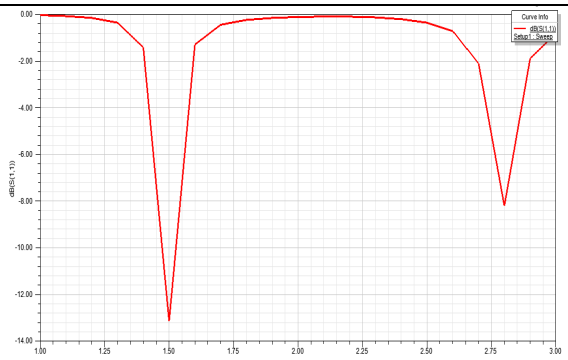

Figure 3. S_{11} Vs frequency plot

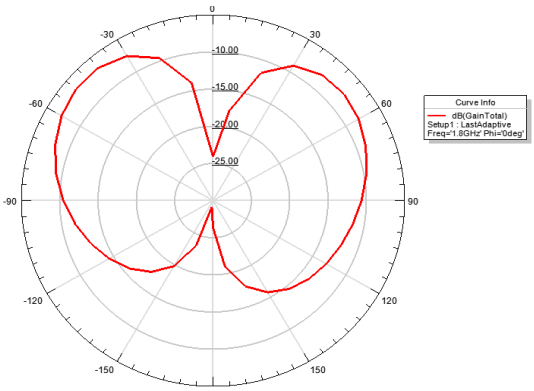

Figure 4. Radiation pattern at 1.8GHz at phi =0deg

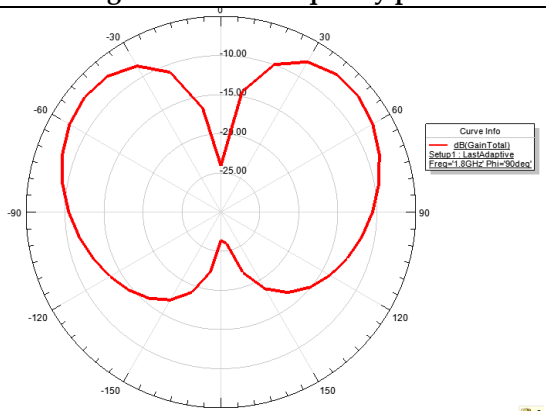

Figure 5. Radiation pattern at 1.8GHz at phi =90deg

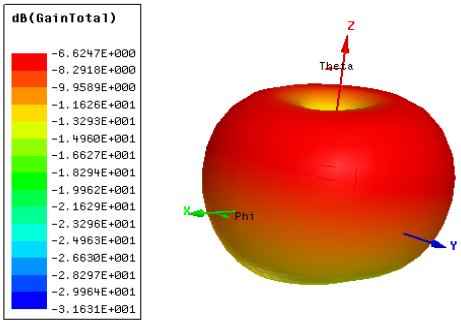

Figure 6. 3D Polar Plot

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RESEARCH ARTICLE

Prediction of Bioactivity of Components of *Curcuma longa* against Giardiasis, through *In silico* Approach

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ABSTRACT

Plants, that occur naturally in plants are useful to them for defense against potential threats from infecting agents and predators. Turmeric (*Curcuma longa*) has gained attentionin worldwide prominence owing to their wide range of medicinal properties. The phytochemicals present in it, though are non-nutritive chemicals, but still have protective and disease preventive properties in them. Researches havealso demonstrated that these phytochemicals can also protect humans against several diseases. Giardiasis is caused by contamination due to *Giardia lamblia*. One of the key proteins, which is involved in its metabolic pathway is Giardia lamblia 15.5 kD RNA binding protein. The molecular docking of the phytochemicals present in *Curcumalonga* was evaluated with the proteinfrom*Giardia lamblia*using BIOVIA Discovery Studio. The strength of the interaction and efficacy was evaluated based on level of-CDocker energy and -CDocker interaction energy. Values that were skewed towards the positive side for both the-CDocker energy and -CDocker interaction energy represented an efficient and stable interaction between the phytochemical and the protein. It was identified that out of different phytochemicals that are present in *Curcuma longa*, Bisdemethoxycurcumin and benzene can efficiently deactivate *Giardia lamblia* 15.5 kD RNA binding protein thereby interrupting the life cycle of *Giardia lamblia*

Keywords: Phytochemical, BIOVIA, Discovery studio, *Curcuma longa,Giardia lamblia.*

INTRODUCTION

Phytochemicals are plant based natural chemical productswhich has several roles to play. Some of them can providecolors to the fruits, flowers, certain others can provide distinctive aroma to them, whereas, certain others are able to provide defense to the plant against potential threats. These phytochemicals can also provide health benefits to human beings on consumption. Phytochemicals, due to this property are often regarded as research

componentalong with the property of being anessential nutrient [1]. They have gained attention as their possible health effects has not yet clearly established.Phytochemists study phytochemicals by extractingthe compounds from the plant, followed by identifying their structure and testing in laboratory models, like cell cultures, *in vivo* studies using laboratory animals and in several*in vitro* experiments[2]. Challenges in the process occurswhile isolating specific compounds in order to determine their structures, for identificationof specific phytochemicals that are primarily responsible for their biological activity[3].Based on the health efficiency of phytochemicals, they arecategorized as essential nutrients, contained naturally in plant extracts. They help plants in acquiring their regular functionscoherently and have also been linked to reduction of several chronic diseases[4]. However, there are convincing evidences suggestingof even more health benefits associated with phytochemicals that still needs to be explored [5].

Curcuma longa, belonging to the family Zingiberaceae, is a rhizomatous herbaceous plant which is traditionally known as turmeric in India. It is popularly used as a spice in Indian cuisine. Awide range of biological properties are associated with this herb, such as, anticancer, antimicrobial,anti-inflammatory activities. It also finds use in free radical scavenging activity[6, 7].The vast diversity of *Curcuma*species is plentily available in India, Thailand and several of the tropical Asian countries. Recent studies have reported that the taxonomy of *Curcuma longa* majorly has specimens from South India[8]. Various other species that areused and sold as "turmeric" in parts of Asia belong to few of the physically similar taxas, with overlapping local names.Curcuma contains many active constituents in it, with overlapping biological activities, such as curcuminoids, vitamins, minerals, phytochemicals, cineole and other monoterpenes.

Giardia lamblia causes infection in humans as cysts which metamorphoses into a trophozoite, that can multiply by binary fission in the intestine of human and can cause diseases like diarrhea. It is an intestinal parasite infecting and causing severe intestinal disease worldwide. In the present study, the efficiency of *Curcuma longa* against the Giardia lamblia 15.5 kD protein was evaluated.

MATERIALS AND METHODS

Software used

Dassault Systemes BIOVIA Discovery studio module was used for carrying out the analysis. It uses CDOCKER, a CHARMm-based docking engine in order to perform flexible and efficient ligand-based docking and to provide docking refinement. Dassault Systemes BIOVIA Discovery studio module was used for carrying out the analysis. It uses CDOCKER, a CHARMm-based docking engine in order to perform flexible and efficient ligand-based docking and to provide docking refinement.

List of phytochemicals

Phytochemicals are the plant- based chemicals, that can stimulate the immune system. Several works have reported*Curcuma longa* to contain phytochemicals such asbenzene, chrysin, bisdemethoxycurcumin, coumarin,guaiazulene. The present study is focused on identifying particular phytochemicalsthat are responsible for inhibiting and controlling Giadiasis.

Protein found in Giardia lamblia

It has been reported that Giardia lamblia 15.5 kD RNA binding protein (protein database code 3O85) is engaged in some of the crucial activities that are required for the survival of this particular microorganism.

Molecular docking

Molecular docking techniquewas used to identify the phytochemicalsin *Curcuma longa*, that can covalently bind with the parasitic protein to successfully inhibit its activity. Dassault Systemes BIOVIA Discovery studio tool was employed for identifying molecular interactions between the phytochemicals and protein structure[9]. In the course

of the process, the sdf files for various phytochemicals that are reported in*Curcuma longa* plant were downloaded. The protein database code of *Giardia lamblia* 15.5 kD RNA binding protein was also identified. In odder to identify the active site of the protein, "receptor cavity" protocol underneaththe "receptor-ligand interaction" menu was selected. Molecular docking approachwas carried out using the CDocker entente of BIOVIA Discovery studiosoftware. In it,the "receptor-ligand interaction" resource was exploited to evaluate the interaction energy. The enzyme molecule was regarded as the receptor molecule and the phytochemicalwas regarded as the ligand molecule. The"-CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" were the choice to estimate the quality of the docking. High positive scoreduring the docking studies werecriterion for good interaction between the small molecule or the ligand and the receptor. Thus, the interactions with high values were the index for screening the major phytochemical that are responsible for curing this disease.

RESULTS AND DISCUSSION

Figure 1 shows the active site of the protein*Giardia lamblia* 15.5 kD RNA binding protein. CDOCK is a molecular dynamics (MD) simulated-annealing-based algorithm, with CHARMm-based docking enginewhich isdeveloped for accuracy. The ligand conformations were obtained by Molecular Dynamic methods.

The estimation of -CDOCKER energy was established on the extent of internal ligand strain energy as well as receptor-ligand interaction energy. -CDOCKER interaction reveals the value of the nonbonded interaction existing between the protein and the phytochemical molecule.The most coherentamong all interactions was chosen based on the positive score of -CDOCKER energy and was also dependent on the minute difference between -CDOCKER energy and -CDOCKER interaction energy.Table 1 shows that *Giardia lamblia* 15.5 kD RNA binding protein interacts with bis-demethoxycurcumin and has the highest positive score of -CDOCKER energy i.e. 30.0939 and a minimum difference i.e. 6.1502 between - C DOCKER interaction energy and - C DOCKER energy followed by benzene, coumarin, chrysin. It was also observed that variance between the - C DOCKER interaction energy and - C DOCKER energy was minimum with Benzene i.e. 2.1069, signifying a stable interaction between the ligand and the receptor. Thus, the results indicated thatbisdemethoxucurcumin, chrysin,benzene, and coumarinhave the potentials to effectively deactivate the *Giardia lamblia* 15.5 kD RNA binding protein. Greater positive values for bisdemethoxycurcumin indicated that it could be the most active component against *Giardia lamblia*. Thus, as per the observations in the present study, the key phytochemicals preventing giardiasis caused by *Giardia lamblia* are bisdemethoxycurcumin and benzene.

CONCLUSION

As it known that *Curcuma longa* plant is an effective medicinal plant. However, its activity against giardiasis is caused by *giardia lamblia*was evaluated in the present study. The study was carried out to provide a theoretical basis of the observation. Using BIOVIA Discovery studio software, molecular docking operation was performed to identify and infer the phytochemical (bisdemethoxycurcumin, benzene, chrysin,guaiazulene and coumarin), that could a significantly interact with the protein. It was found that bisdemethoxycurcuminand benzene can form strong bond with the protein and could successfully inhibit the metabolic activities that are associated with the parasite. Thus, this study could explain that the presence of bisdemethoxycurcumin and benzene provided medicinal values to *Curcuma longa*against giardiasis that is caused by *Giardia lamblia*.

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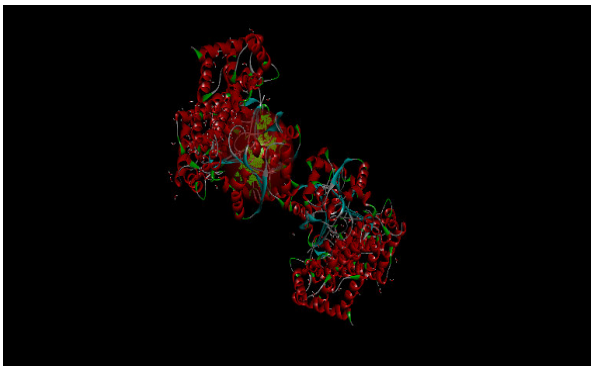

Figure 1. Active site of *Giardia lamblia* 15.5 kD RNA binding protein

Table 1. Results of CDocking of phytochemicals with *Giardia lamblia* 15.5 Kd RNA binding protein

SL NO	LIGAND	- C DOCKER ENERGY	- C DOCKER INTERACTION ENERGY	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	Bisdemethoxy curcumin	30.0939	36.2441	6.1502
2	Coumarin	17.5158	20.7682	3.2524
3	Benzene	10.3898	12.4967	2.1069
4	Chrysin	22.8074	28.8493	6.0419
5	Guaiazulene	-62.5974	22.7445	-85.3419

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RESEARCH ARTICLE

In silico Antifungal Analysis of Bioactive Compounds from *Syzygium aromaticum* against Vulvo-Vaginal Candidiasis

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ABSTRACT

The mixture of a substance with another substance results in blend. The compatibility of 12cd-Glucose and Dichloro-Ethylene were studied to form a mixable blend using Biovia Materials Studio. The miscibility of the two substances was demonstrated on free energy of mixing, chi parameter, phase diagram and mixing energy. The results stipulated that the pair can become congruent at both low and high temperature. Phase diagram specify that a single phase can be obtained above 387.5K which was the critical temperature. The mechanical properties of the composite were reviewed based on bulk modulus, shear modulus, Young's modulus, Poisson ratio and brittle stress fracture. The results indicated that the values of all the properties increased with increase in mass fraction of dichloro-ethylene. The composition of the blend was examined with respect to heat capacity, thermal conductivity and dielectric constant which are permeability properties. The molar volume and density decreased with increase in dichloro-ethylene fraction. The permeability properties of the composite were studied based on permeability of oxygen, nitrogen and carbon dioxide. The results showed that the permeability for all the gases decreased with increase in mass fraction of dichloro-ethylene. This study will not only help to determine pairs without performing laboratory experiments but also less time consuming and low cost process.

Keywords: phytochemical, BIOVIA, Discovery studio, *Syzygium aromaticum*, *Candida.*

INTRODUCTION

Since primeval times, the mankind is largely dependent on plants for treating common diseases and many of these traditional techniques are still included as part of the routine treatment of many maladies [1]. Folk medicine, having originfrom plants, are currently gaining regards due to their natural originspecially in the developing countries, where modern health services is still limited. However, in the absence of a scientific evidence, such medication is

seen with a suspicion of having serious adverse effects. Hence the thorough evaluation of the pharmacological activity of herbal extract therefore needs to be designed to make its use in economically unprivileged regions [2].In the current past, use of plant extracts and other forms of alternative medicine has gained much attention worldwide. Clinical microbiologists look forward at plant-based medications as antibioticscan be formulated form such medication and also because many of these medications are commonly available [3].In addition, overuse of several drugshas caused appearance of many resistant microbial strains so alternative medicines have become a need in the current situation [4].

In India, use of indigenous systems of medicine like Ayurveda, Unani and Sidha has never diminished. Ayurvedic texts like the 'Charak Samhita', 'Sushrut Samhita', 'Bhavaprakasha Samhita', 'Satmya Darpan Samhita', 'Sarangadhara Samhita', 'Vaisajya Ratnabali,' 'Rasatarangini' have explained numerous remedies for treating several ailments. In fact, many plant-based medications are still in demand for treating variety of diseases like inflammatory conditions, arthritis, bronchitis, tuberculosis, congestive cardiac failure, cancer, etc. The medicinal value of the plants lies in the chemical substances present in them, that can produce distinct physiological effect on human body, these substances are called phytochemicals,which have gained attention for their therapeuticefficiency. Plants based medicinal composition can be derived from all parts of plant such as their barks, leaves,roots, flower, fruits, and seeds. Various medicinal plants with their phytoextracts are reported to have numerous medicinal qualities, like anti-microbial, anti-diabetes, anti-oxidant, anti-inflammatory,anti-cancer, etc [5].Clove belonging to the family of Myrtaceae,can be used to cure disease like candidiasis and certain other infections due to its medicinal properties. Clove is known to contain phytochemicals such aseugenol, gallic acid, kaempferol, β-caryophyllene, campestrol, myricetin, oleanoic acid, vanillin, rhamnetin and stigmasterol. There is a greater probability that the medicinal value of clove owes to several of the phytochemicals present in it[6]. However, there are notmany reports identifying the specific phytochemical responsible for the cure of candidiasis.

Fungal infections are a common disorder, effecting people commonly throughout the world. Particularly rural areas of developing nations are affected by it, due to improper sanitation, insufficient dietary food and supplements, etc, as fungal infections can affect people in all age groups. A group of fungi belonging to the genus Candida generally cause Candidiasis. Candida fungus typically habitatsthe skin, gastro-intestinal tractand vagina and sheds through vaginal secretions. Humans become infected most frequently by this decrease due to antibiotics, poor eating habits, hormonal imbalance near menstrual period, stress, lack of sleep, weak immune system.This study focuses on the identification of the phytochemical from*Syzygium aromaticum*that are responsible to cure Candidiasis caused by *Candida sp.*

MATERIALS AND METHODS

Software used

Dassault Systemes BIOVIA, Discovery studio was used for analysis in the current study. It is a new formulation for conducting predictions for biologics, that utilizes machine learning techniques in order to predict the level of molecular interaction between the ligand and the enzyme.

List of phytochemicals

Phytochemicals are secondary metabolites that are produced by plants, which have protective effects in them. On absorption of these phytochemicals, they provide immunity against bacteria, viruses, fungi, etc. Reports have suggested that *Syzygium aromaticum*contains phytochemicals such as eugenol, gallic acid, kaempferol, β-caryophyllene, campestrol, myricetin, oleanoic acid, vanillin, rhamnetin and stigmasterol. It has been established that *Syzygium aromaticum*plant belonging to Myrtaceae family has potential to help control Candidiasis. This work is focused on identification particular phytochemicals from *Syzygium aromaticum*that could be responsible for inhibiting and controlling of Candidiasis.

Enzyme found in *Candida*

It has been reported that candidiasis can be caused as a result of *Candida sp.* infestation[7]. Variousmetabolic cycles are required by fungi for its survival. These metabolic cycles are regulated by several enzymes. RCSB enzyme database was screened for identifying and listing different enzymes essential for the metabolic pathways in *Candida sp.* fungus. It was found that enzyme dihydrofolate reductase (protein database code 3QLW) is involved in a mechanismwhere it catalyses the transfer of hydride to dihydrofolate from NADPH, this is accompaniedby protonation to produce tetrahydrofolate, which is very crucial for survival of this microbe.

Molecular docking

Here, molecular docking method was used for identifying phytochemicals from plant extract, that could act as ligand to form strong covalent bond with the fungal protein and inhibit it. The Dassault Systemes BIOVIA, Discovery studio software was used for identifying the strength of molecular interaction and for performingthe molecular docking. At first the sdf files for the phytochemicals present in *Syzygium aromaticum* were downloaded from pubchem. The protein database code of the dihydrofolate reductase enzyme was downloaded from the RCSB site. For the identification of the active site of the enzyme "receptor cavity" protocol present under "receptor-ligand interaction" menu was used. Molecular docking was carried out using C-Docker protocol of Dassault Systemes BIOVIA, Discovery studio software. The phytochemical was treated as the small molecule or the ligand molecule and the enzyme was treated to be the receptor molecule.

The "-CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" were obtained and analysed for the better understanding of the quality of molecular docking. High positive value of "-CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" indicated good and stable interaction between the ligand and the receptor. Thus, interaction with high values indicate major phytochemical responsible for curing the disease.

RESULTS AND DISCUSSION

Figure 1 shows the active site of dihydroxyfolate reductase (protein data base 3QLW) docked with phytochemicals present in *Syzygium aromaticum*(clove), which appears green in color. C-DOCK is a molecular dynamics (MD) simulated-annealing-based algorithm, which is a grid-based molecular docking method that is optimized for accuracy. The ligand conformations were obtained by Molecular Dynamic methods. -CDOCKER energy was calculated based on the internal ligand strain energy and receptor-ligand interaction energy. -CDOCKER interaction implies to the energy of the non-bonded interaction existing between the protein and the ligand. The best and stable interaction were chosen based on a) high positive value of -CDOCKER energy and b) small difference between -CDOCKER energy and -CDOCKER interaction energy [8]. Table 1 shows that the interaction between dihydrofolate reductase and kaempferol; dihydrofolate reductase and Myricetin; dihydrofolate reductase and Rhamnetin; dihydrofolate reductase and Vanillin has positive value of -CDOCKER energy and minimum value of the difference between - C DOCKER interaction energy and - C DOCKER energy followed by myricetin.

Thus, the results indicated that kaempferol and myricetin can effectively deactivate the enzyme thereby interrupting the biological cycle of *Candida sp*. On the other hand beta-caryophyllene, eugenol, rhamnetin, vanillin deactivate the enzyme to a certain extent. Stigmasterol, campestrol, gallic acid, oleanoic acid cannot interact with dihydrofolate reductase enzyme. Thus, the key phytochemicals preventing candidiasis infection caused by *Candida sp.* are kaempferol, myricetin, Rhamnetin and Vanillin.

CONCLUSIONS

It is known that *Syzygium aromaticum* plant has medicinal action against candidiasis, which is caused by *Candida sp*[9]. This study was carried out to provide the theoretical basis for this observation. Using Dassault Systemes BIOVIA, Discovery studio software, molecular docking was performed to identify the phytochemical that can have a

significant interaction with the vital enzyme (dihydrofolate reductase) of the microbe. It was found thatare kaempferol, myricetin, Rhamnetin and Vanillin can form strong bond with the enzyme and successfully inhibit the metabolic cycle of the microbe, explaining that these phytochemicalscanprovide medicinal values to *Syzygium aromaticum* against Candidiasis caused by *Candida Sp.*

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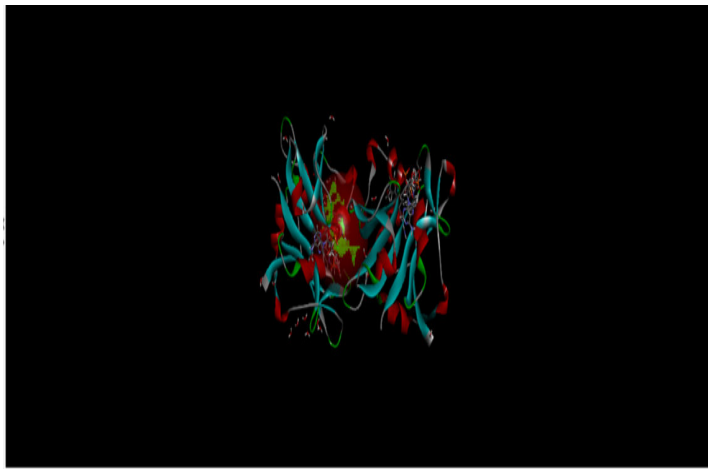

Figure 1. Active site of dihydroxyfolate reductase enzyme

Table 1. Results of C-Docking of phytochemicals with dihydrofolate reductase (receptor)

SL NO	LIGAND	- C DOCKER ENERGY	- C DOCKER INTERACTION ENERGY	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	β-Caryophyllene	-21.8776	21.0401	42.9177
2	Campestrol	Failed	Failed	NA
3	Eugenol	10.7172	20.8951	10.1779
4	Gallic acid	Failed	Failed	NA
5	Kaempferol	22.7256	28.003	5.2774
6	Myricetin	22.6612	26.7662	4.105
7	Oleanoic acid	Failed	Failed	NA
8	Rhamnetin	20.9616	27.3538	6.3922
9	Stigmasterol	Failed	Failed	NA
10	Vanillin	14.9155	18.5368	3.6213

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RESEARCH ARTICLE

Study of Antifungal Activity of Phytochemicals from *Azadirachta indica* against Vulvo -Vaginal Candidiasis: An *In silico* Approach

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ABSTRACT

Medicinal plants have wide potentials in treating a variety of infectious as well as non-infectious diseases. The worthiness of plants in treating disease have increased eventually due to the resistance of several microorganism towards several synthetic antibiotics. Most of these antibiotics are also associated with toxicity and side effects during prolonged treatment. Due to these reasons medicinal plants are considerably used by most of the traditional medical practitioners for the purpose of curingdiseases in their day to day practice. Phytochemicals are biologically active compounds that are obtained from plants. It has been reported that *Azadirachta indica*plant extract has several medicinal values, including the treatment of candidiasis. The plant extract is enriched withseveral phytochemicals, that attribute towards the potential effects in *Azadirachta indica*. One of the key enzymes involved in the biochemical pathway of Candidiasis which is caused by *Candida sp*is dihydrofolate reductase. Molecular docking approach for the phytochemical screening of *Azadirachta indica*against this enzyme was evaluated using BIOVIA Discovery Studio. The strength of the interaction between the ligand and the enzyme was evaluated based on -CDocker energy and -CDocker interaction energy. Positive values during the analysis indicated that phytochemicals L-ascorbic acid and oleic acid can effectively deactivate the enzymedihydrofolate reductase and interrupt the life cycle of *Candida.*

Keywords: phytochemical, BIOVIA Discovery studio, *Azadirachtaindica,Candida.*

INTRODUCTION

Several plants have found usesfor their therapeutic properties, since the primeval times. Based on these properties, variety of drugs have been obtained from medicinal plants. More than 80% of individuals from developing countries depend on plant-basedformulationsand traditional medicinal system for their primary health care [1].Plants have a potential to produce diverse range of bioactive constituents and hence qualify as arich sourceforseveral types of therapeutic applications[2]. Mostly, these phytochemical compounds are secondary metabolites liketannins,

flavonoids, alkaloids, steroids, resins, fatty acids, phenol compounds, etc. Due to the presence of these metabolites, extracts from various parts of the plants can treat ailments likecough, cold, fever, diarrhoea, dysentery, bronchitis, cholera, etc. [3]. Even, plant derived products have found advantage due to easy availability, effectiveness of the compound, less side effects and reduced cost [4].Presently, antibiotic resistance in medically relevant microbes is of major concern that is faced by the world. Also, the indiscriminate use of synthetic antimicrobial drugs has caused multiple drug resistance. Moreover, antibiotics at times can cause adverse effects on the hostsimmunity such ashypersensitivity, allergies, immune-suppression, etc. This has sparged the need to develop an alternative to synthetic drugs for the treatment of infectious diseases[5].

Therapeutic plants have enormous potentials in the treatment of infectious diseases and can simultaneously minimize side effects that are often associated with synthetic drugs [6]. Neem belonging to the family Meliaceae, is used to cure several diseasesincluding candidiasis[7]. It is known to contain phytochemicals such asnimbin, oleic acid, beta-sitosterol, glutamic acid, lactose, L-ascorbic acid, maltose, stigmasterol [8]. Certain phytochemicals present in neem, play an essential role in curing candidiasis. However, there is not much identification of the specific phytochemical responsible to cure candidiasis. Candidafungus typically invades the human gastro-intestinal tractalong with the skin and vagina and infects the intestinal tract, skin, as well as the vagina[9]. Present study focuses on the identification of phytochemicals from*Azadirachta indica*that are helpfulin the cure forCandidiasis caused by *Candida sp.*

MATERIALS AND METHODS

Software used

Dassault Systemes BIOVIA, Discovery studio was used for studying the molecular docking between the ligand and the enzyme. This software makes use of machine learning approachfor predicting the levels of molecular interaction among the molecules.

List of phytochemicals

Phytochemicals are compounds produced by plants as secondary metabolites that helps them thrive pathogens, competitors predators. Studies have suggested that consuming foods and beverages, that are rich in phytochemicals helps prevent diseases. Several works have also reported that *Azadirachtaindica*containinglactose, L-ascorbic acid, maltose, beta-sitosterol, glutamic acid, nimbin, oleic acid, stigmasterol, etc has many therapeutic applications. It has also been established that *Azadirachtaindica*plant belonging to Meliaceae family has potentials even to control the infection caused byCandidiasis. The present study is focused on identifying the phytochemicals particularly responsible for inhibiting and controlling of Candidiasis.

Enzyme found in Candida

It has been reported that candidiasis can be caused as a result of *Candida sp.* infestation. Several metabolic pathwaysare involved in the fungal life cycle for their survival. For the regulation of these metabolic cycles,many enzymes get involved in their pathway. RCSB enzyme database was used to screen and list different enzymes associated with*Candida sp.*Dihydrofolate reductase enzyme (protein database code 1M78) was selected for this study. This enzyme in general is involved in DHFR catalyses by transfer of hydride from NADPH to dihydrofolate with an accompanying protonation to produce tetrahydrofolate.

Molecular docking

Molecular docking was carried out to identify the stable interaction between the phytochemical from the plant extract and the fungal enzyme. The identified phytochemicals act as ligand and were screened for their stable interaction with the fungal protein by forming covalent bond in order to successfully inhibit the microbe. Dassault

Systemes BIOVIA, Discovery studio was used for identifying molecular interaction and performing molecular docking. For the analysis, the sdf files of the phytochemicals found in the *Azadrichata indica*plant were downloaded from PubChem. For the protein database code for dihydrofolate reductase enzyme, RCSB site was preferred. During the docking, active site of dihydrofolate reductase was identified by using "receptor cavity" protocol present in "receptor-ligand interaction" menu of BIOVIA Discovery Studio. Molecular docking for interaction energy was evaluated using the CDocker protocol under "receptor-ligand interaction". The enzyme dihydrofolate reductase was treated asreceptor and the selected phytochemicals were treated as the small molecules or ligands. The values of "-CDOCKER_ENERGY" as well as "-CDOCKER_INTERACTION_ENERGY" were used for identifying for the quality of docking and interaction. Results withgreater positive values indicated the presence of a good interaction between the ligand and the receptor and a lesser difference between "CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" indicated a stable interaction. Thus, the interactions with high values suggested the phytochemical responsible for curing of Candidiasis.

RESULTS AND DISCUSSION

Figure 1 shows the active site present in dihydrofolate reductase enzyme, which appears light green color. CDOCK is a molecular dynamics (MD) method that predicts the molecular interaction between the small molecule and the targeted protein, by using simulated-annealing-based algorithm. -CDOCKER energy was calculated for the study was analysedbased on the internal ligand strain energy as well as receptor-ligand interaction energy. -CDOCKER interaction implies the energy of the non-bonded interaction which exists between a ligand and a protein. The most efficient interaction among all interactions was selected based on a) greater positive value of -CDOCKER energy and b)minimum difference between -CDOCKER energy and -CDOCKER interaction energy [10].From the present study, it was observed that Table 1 shows that dihydrofolate reductase-Oleic acid interaction has the highest positive value of -CDOCKER energy(35.2949) and minimum value of the difference (15.1433) between - C DOCKER interaction energy and - C DOCKER energy followed by L-ascorbic acid. Thus, the results indicated that Oleic acid and L-ascorbicacid can have some deactivatingeffect ondihydrofolatereductase enzyme and are able to interrupt the biological cycle of *Candida sp.*to some extent. Maltose, nimbin, stigmasterol, lactose, glutamic acid cannot interact with dihydrofolate reductase enzyme. Table 1. Results of CDocking of phytochemicals with dihydrofolate reductase (receptor)

CONCLUSIONS

It is already known that*Azadrichata indica*has immense medicinal potentials. In the present study we have tried evaluating its efficiency in treating candidiasis, which is caused by *Candida sp.* This study was carried out in an attempt to provide theoretical basis of this observation. Using Dassault Systemes BIOVIA, Discovery studio, molecular docking operation was performed to identify the phytochemical that could have some activity against the vital enzyme (dihydrofolate reductase) of the microbe. It was found that Oleic acid and L-ascorbic acid can form interaction with the enzyme and inhibit its metabolic cycle to some extent whereas, nimb, lactose, stigmasterol, maltose and glutamic acidcannot deactivate the enzyme. Thus, this study could explain that the presence of Oleic acid and L-ascorbic acid provided the medicinal values to *Azadrichata indica*against Candidiasis caused by *Candida Sp.*

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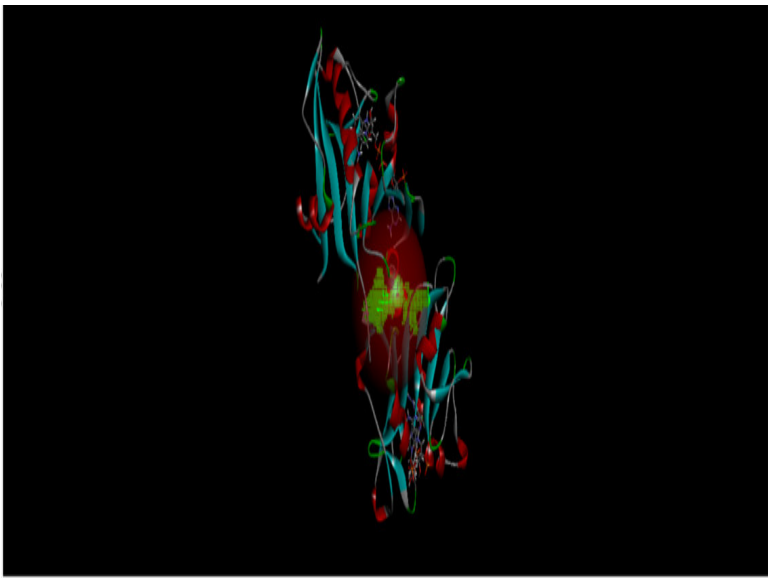

Figure 1. Active site of dihydrofolate reductase enzyme

Table 1. Results of CDocking of phytochemicals with dihydrofolate reductase (receptor)

SL NO	LIGAND	- C DOCKER ENERGY	- C DOCKER INTERACTION ENERGY	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	Oleic acid	20.1516	35.2949	15.1433
2	L-ascorbic acid	4.61256	21.5129	16.90034
3	β-sitosterol	-41.8324	31.9759	73.8083
4	Stigmasterol	Failed	Failed	NA
5	Maltose	Failed	Failed	NA
6	Nimbin	Failed	Failed	NA
7	Lactose	Failed	Failed	NA
8	Glutamic acid	Failed	Failed	NA

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RESEARCH ARTICLE

Screening of Phytochemicals of *Aloe barbadensis miller* for its Anti-Inflammatory Activity against Rheumatoid Arthritis: An *In Silico* approach

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ABSTRACT

The secondary bioactive components in plants are known asphyotochemicals. It has been reported that such phytochemicals have therapeutic propertiesthat have shown tremendous potentials in treating several diseases. Rheumatoid arthritis, which is a chronic, progressive, disabling autoimmune disease, that is characterized by systemic inflammation occurring in the joints, has gained importance due to its increased occurrence based on the current lifestyle adaptation by majority of the people. It is a systemic disease which means, it can affect the entire. Medicinal properties of several herbs and plants in various forms have shown reliving effectsin the pain and inflammation in joints, caused due to Rheumatoid arthritis. Several reports have shown that phytochemicals such as Aloe vera has therapeutic action against Rheumatoid Arthritis (RA). The enzymatic pathway involved in Rheumatoid arthritis include several functions associated with cyclooxygenase enzyme. In the present study, molecular docking of the phytochemicals that are present in *Aloe barbadensis miller* was carried out with the enzymecyclooxygenase using BIOVIA Discovery Studio. The strength of the interaction and its efficacy was interpreted based on the values of -CDocker energy and -CDocker interaction energy obtained in the docking. Values that were skewed towards the positive side for both CDocker energy as well as -CDocker interaction energy indicated that among the various phytochemicals evaluated,Salicyalic acid can effectively deactivate cyclooxygenase interrupt with its enzymatic activity

Keywords: Phytochemical, BIOVIA, Discovery studio, cyclooxygenase, Rheumatoid Arthritis.

INTRODUCTION

The medicinal values of these plants lie in the chemical substances present in them, that have definitive physiological effect on human body [1].Medicinal plants, since time worn, have been used in all intent and purpose as a source ofmedicine. It isestimated that approximately 80- 85% of population both in developed as well as developing nations rely on traditional therapeutics for primary health care needs. It ispresumed that a major part of thecustomary therapy involves use of plant extracts as the activeingredient [2].

Since ages various ailments and infectious disease have found remedies by use of herbal constituents throughout the world. Thus, scientists are considerably turning their attention to natural products, either in the form of pure compounds or in the form of standardized plant extracts, in search for new leads towards developing better drugs against several diseases [3]. Pathogenic microoganismsleadto a number of diseases by invading into the organs or throughtoxigenesis. Synthetic antibiotics although are effective in treating such diseases, but they still could cause oxidative stress leading to damage of DNA, proteins and lipids in human cells. Thus, medicinal plants have emerged as an alternate to theuse of synthetic drugs, as they contain phytochemicals and antioxidants that could tile the way towards development of antimicrobial drug, curative in cancer therapy[4]. But now a days due to our bad and unhealthy food habit and life style a list of life style related diseases are arising gradually like high blood press, diabetes, arthritis etc.

Rheumatoid arthritis (RA) is a systemic disease that manifests rheumatoid nodules, vasculitis, eye inflammation, cardio pulmonary disease[5]. Rheumatoid arthritis is not an inherited disease. Researchers believe that some people developed genes that make them susceptible towards this disease. People with such susceptible genes will however not automatically develop rheumatoid arthritis. There occurs a "trigger," such as an infection or some environmental factor, which activates this gene. When the body is exposed to such triggers, the immune system responds inappropriately. Instead of protecting the joint, the immune system itself initiates to produce substances that could attack the joints. Hence, RA is an autoimmune disease which means that the body's immune system mistakenly attack on its healthy tissues in case of RA. The normal joint lining is usually thin and has very few blood vessels in it but in caseofRA, joints lining becomes thick and crowded with white blood cells. These white blood cells secrete chemical such as interleukin-1 (IL-1) and tumor necrosis factor alpha (TNF-alpha) that cause joint swelling, damage and pain in the joints [6].

Rheumatoid arthritis is a chronic inflammatory condition affecting the bone joints causing swelling, pain and stiffness that can gradually lead to the substantial loss of functioning and mobility in advanced stages [7].High levels of immunoreactive cyclooxygenase (Cox; prostaglandin H synthase) are present in the synovia of patients suffering from rheumatoid arthritis[8]. Effects of RA are not only limited to extreme physical distress but they can also cause mental distress in the patients suffering from it. As the etiology behind RA prognosis is clearly understood, confirmed curative measures are not developed till date. All current treatment regimens and therapies such as cytokine therapy (anti-TNFα therapy) or Disease Modifying Anti-Rheumatic Drugs (DMARDs) are limited to reduction of its symptoms and to delay its pathogenesis. Thus, RA has become an undeniable threat to human life, for which preventive measures must be developed sooner [9].

In the recent times, a large array of research is directed towards the search for herbal solutions to the treatment of the diseases. In Indian Ayurveda, one such promising herbal candidate that has anti-arthritic effect is *Aloe vera* (Family Xanthorrhoeaceae), a perennial succulent xerophytic plant. *Aloe vera* has been used for many centuries for its curative and therapeutic properties [10]. In this plant water gets held in the form of viscous mucilage within its thin walled parenchymatous cells that are located in the innermost part of the leaves. *Aloe barbadensis miller*is cultivated in Europe and also in several parts of India, including north-west Himalayan region. Aloe vera is considered to be among the important plants used in folk medicine. Anthraquinone, anthracene, cinnamic acid and anthranilic acid are some important constituents present in it, that are responsible for its activity. Aloe vera is used in variety of skin

ailments such as mild cuts, bruises, insect stings, eczema, poison ivy. It has antibacterial and antifungal properties, which is implied for blood purification, anti-inflammatory activity, diuretic, uterine tonic, spermatogenic, laxative, purgative activity and fever reliever. Aloe vera is able to stimulate the immune system and is hence a powerful anti-inflammatory agent[11, 12]

Aloe vera gel is traditionally consumed or applied dermally to reduce the pain caused in joints. Phytochemical screening of *Aloe vera* confirms the presence of flavonoids, alkaloids, resins, tannins, steroids, etc in it[13].The anti-arthritis property of aloe vera is attributed to the presence of anthraquinone compound in it [14].*Aloe vera* is a perennial, drought-resisting, succulent plant that belongs to Asphodelaceaefamily. The name,aloe, is derived from the Arabic "alloeh" or Hebrew "halal" meaning bittershiny substance. It has a crucial role in indigenous system of medicine such asayurveda,unani, siddha, and homoeopathy [15].*Aloe Vera* or the Sanskrit name "Ghee kunwar" has lance-shaped, sharp pointed and jagged & edged leaves. It is found as a wild herb along the coast of south India. It is under cultivation in fairly large areas in many parts of India viz; Tamil Nadu, Gujarat, Maharashtra etc [16].

MATERIALS AND METHODS

Software used

For the evaluation of the interaction, Discovery studio module of BIOVIA software (Dassault Systemes of France) was used. This software makes use of machine learning techniques for predicting the level of molecular interaction between the ligand and the enzyme.

List of phytochemicals

Phytochemicals are plant based secondary metabolites that enables protection from predators. These plant components on consumption provides immunity to ward off several diseases in humans, hence they are also utilized in the form of traditional medicine. Published works have reported*Aloe barbadensis miller*to contain Salicyalic acid,Aloinin it, which have shown several beneficial effects. It has already been established that *Aloe barbadensis*plant belonging to familyAsphodelaceae has potential in controlling Rheumatoid arthritis. The current study is focused on identification of the particular phytochemical responsible for inhibiting and controlling Rheumatoid arthritis in patients.

Enzyme Responsible for Rheumatoid arthritis (RA)

Rheumatoid arthritis can be caused as a result of several enzymatic pathways leading to bone erosion.These enzymatic pathwaysrequire the use of various enzymes to play crucial role in causing the disease. For the identification and screening of the enzyme crucial for Rheumatoid arthritis, BRENDA enzyme database was used. It was found that cyclooxygenaseenzyme (protein database code 3N8Y) is involved in some major pathways associated with rheumatoid arthritis.

Molecular docking

Molecular docking using C Docking method was carried out to identify the phytochemicals from *Aloe barbadensis miller*, that could probably act as ligand to form strong covalent bond with the human protein and inhibit it. The Discovery studio module of BIOVIA software was used for evaluating the molecular interaction by molecular docking. During the process, the sdf files for the particular phytochemicals from*Aloe barbadensis miller* plant were downloaded. The protein database code of cyclooxygenase enzyme was also identified. For identification of the active site of the enzyme “receptor cavity” protocol under "receptor-ligand interaction" menu was used. Molecular docking was carried out using the CDocker protocol under “receptor-ligand interaction”. The phytochemical was considered as the small molecule or the ligand that interacts with the enzyme, which was considered as the receptor molecule.The“-CDOCKER_ENERGY” and “-CDOCKER_INTERACTION_ENERGY” were used as indicator for the

quality of molecular docking. High positive values obtained during the docking studies indicated good interaction between the ligand and the receptor. Thus, the interactions with high values owed to the major phytochemical that were responsible for curing the disease.

RESULTS AND DISCUSSION

Figure 1 shows the active site of the enzymecyclooxygenase, that appears light greenin color. CDOCK is a molecular dynamics (MD) simulated-annealing-based algorithm, which is grid-based molecular docking technique and is optimized for accuracy. The ligand conformations for this study were obtained by Molecular Dynamic methods.-CDOCKER energy was calculated on the basis of internal ligand strain energy and receptor-ligand interaction energy. -CDOCKER interaction signifies the energy of the nonbonded interaction existing between the protein and the ligand.The most efficient interaction of the ligand with the protein was screened on the basis of the positive value of -CDOCKER energy and small difference between -CDOCKER energy and -CDOCKER interaction energy [17].

Table 1 shows that interaction ofcyclooxygenase with several phytochemicals, out of which salicyalic acid has the highest positive value of -CDOCKER energy i.e. 18.86 and a minimum difference between - C DOCKER interaction energy and - C DOCKER energy i.e. 3.2. This wasfollowedby Aloin. Thus, the results indicated that salicyalic acid can effectively deactivate thecyclooxygenase enzyme thereby interrupting the biological enzymatic pathway associated with rheumatoid arthritis. Higher positive values for salicyalic acid indicated that it was the most active component against cyclooxygenase. Thus, the key phytochemicals preventing Rheumatoid arthritis areSalicyalic acid and Aloin.

CONCLUSION

Aloe barbadensis miller is a popular medicinal plant. The phytochemicals from this plant was assayed against Rheumatoid arthritis. Rheumatoid arthritis is caused by cyclooxygenase. This study was carried out to provide a theoretical basis to this observation. Using Discovery studio BIOVIA software, molecular docking operation was carried out to identify the phytochemical (salicyalic acid,aloin) that showed a significant interaction with the enzyme. It was found that both can form strong bond with the enzyme and can successfully inhibit its enzymatic pathway. Thus, this study could explain the role ofsalicyalic acid and aloinin providing medicinal values to *Aloe barbadensis miller* against Rheumatoid arthritis.

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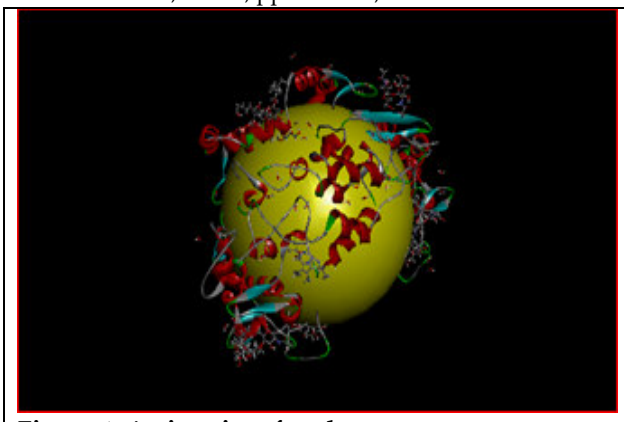

Figure 1. Active site of cyclooxygenase

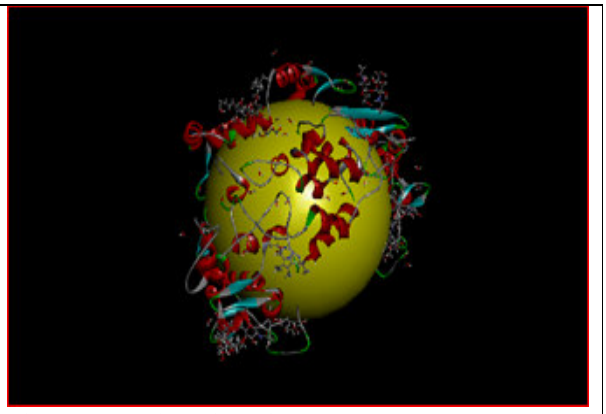

Figure 1. Active site of cyclooxygenase

Table 1. Results of CDocking of phytochemicals with cyclooxygenase

SL NO	LIGAND	- C DOCKER ENERGY	- C DOCKER INTERACTION ENERGY	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	Salicyalic acid	18.86	22.06	3.2
2	Aloin	14.60	56.82	42.22

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RESEARCH ARTICLE

In silico Methodology for Phytochemical Analysis of *Azadirachta indica* against Rheumatoid Arthritis

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ABSTRACT

Phytochemicals are non-nutritiveplant-based compounds, which are considered to show efficiency against several pathogens. *Azadirachta indica* popularly known as Neem has several medicinal effects. In the current study, the plant extract was studied for drugs like properties against rheumatoid arthritis. One of the key enzymeinvolved in rheumatoid arthritis is cyclooxygenase (COX2) which causes joint destruction in rheumatoid arthritis.The extracts from neem plant contains different phytochemicals which were studied for their activity against cyclooxygenase. The molecular docking of the phytochemicals with the enzyme was studied using BIOVIA Discovery Studio. The strength of the interaction was evaluated based on -CDocker energy and -CDocker interaction energy. The high positive interaction energy of the phytochemical can be considered to be due toits effectiveness on enzyme. Out of different phytochemicals Anthelmintic and ethyl acetate shows the high positive interaction against the enzyme. So these two phytochemicals can be concluded to be able to deactivate the enzyme.

Keywords: Phytochemical, BIOVIA, Discovery studio, cyclooxygenase, Rheumatoid Arthritis

INTRODUCTION

The current health conditions when compared to the previous days seems to be deteriorating to a larger extent.Previously, the lifestyle was dependent on the natural environment andwas comparatively healthier. Today, the modern life style, is fast paced, comfortable, stressful and unhealthier. Changing work condition, decrease in physical activity, sedentary jobs types, comfortable but stressful life along with bad eating habits has exposed us to some dangerous health hazards like blood pressure, diabetes, obesity etc. If caution and changes in lifestyle are implemented, we can prevent these lifestyle related diseases from increasing further.Nature is animmense source of medicinal agents for millions of years. Many pharmaceutical industries are dependent on natural sources for production of modern drugs. Even in the current era, we are highly dependent on traditional medicine.Nutraceuticals have also gained significance with the increasing demand for health supplements, as

nutraceuticals are nutritionally or medicinally enhanced foods, that have health benefits. They include engineered grains; cereals supplemented with vitamins and even minerals or genetically manipulated soybean and canola oil without trans fatty acids[1, 2].The WHO estimates that approximately 80% people rely on traditional medicine for their primary health care needs. Since medicinal plants are the 'backbone" of traditional medicine, hence majority of people are reported to dependon medicinal plants on a regular basis [3]. The medicinal value of the plants lies in some chemical substances that are present in it and can produce a definite physiological action on the human body, such substances are called phytochemicals, and have therapeutic applications. Plants based therapeutic components can be derived from any part of plant like bark, leaves, flowers, roots, fruits, and seeds [4]. Various medicinal plants and their phytoextracts are reportedto have numerous therapeuticbenefits like anti-microbial, anti-diabetes, anti-oxidant, anti-inflammatory, anti-cancer, etc. [5]. Many of the medicinal plants are used as spices and food items, they also have applications as medicines like allopathic medicine, herbal medicine, alternative medicine, homoeopathy and aromatherapy [6].Among different sources of natural products, plants have been a source of novel chemical substance, which serves as starting materials for a number of old and new pharmaceutical products. Plants that demonstrated efficiency such as anticancer, antioxidant, anti-inflammatory, immunostimulatory and antimicrobial properties have received research attention.

In the current study, *Azadirachtaindica*that belongs to family Meliaceae was used to choosen to study its effectiveness against Rheumatoid arthritis.Rheumatoid arthritis is a chronic inflammatory disease which causes joint destruction. It is reported that Cyclooxygenase enzyme causes the increase in prostaglandin synthesis at the infection site. Cyclooxygenase (COX-2) is known to be upregulated *in vitro* by inflammatory agents, like lipopolysaccharide, IL-1 and TNF [7]. The phytochemicals of *Azadirachtaindica* are reported to be anthelmintic, nimbin, nimbinin, nimbidin, ethyl acetate, petroleum ether. etc. There is high possibility that these phytochemicals play a major role in curing join infection in arthritis. However, there is no report identifying the specific phytochemical responsible to cure arthritis. Hence the current study helps in identifying the phytochemicals that have specific activity against Rheumatoid arthritis.

MATERIALS AND METHODS

Software used

Discovery studio module of BIOVIA software (Dassault Systemes of France) was usedfor docking inthe present study. This software utilizes machine learning techniques in order to predict the level of molecular interaction taking place between the ligand and the protein molecule.

List of phytochemicals

Phytochemicals are produced by plants as secondary metabolites to protect them from predators. These phytochemicals show potential activity against several bacteria, viruses, fungi etc.When these plants or their parts are consumed, their phytochemicals help fight off threats to the health. All parts of *Azadirachtaindica* i.e. its leaves, flowers, seeds, fruits, roots and bark are used traditionally for the treatment of infections,skin diseases,inflammation, dental disorders, etc. As this plant has immunomodulatory, anti-inflammatory, antihyperglycaemic, antiulcer, antimalarial, antifungal, antibacterial, antiviral, antioxidant, antimutagenic and anticarcinogenic properties[8].*Azadirachta indica* contains various phytochemicals such as Anthelmintic, Nimbin, Nimbolide,ethyl acetate, petroleum ether, Azadiradione, etc which were all studied to analyse their activity against Rheumatoid arthritis.This study was focused on identification of the particular phytochemical responsible for inhibiting and controlling of rheumatoid arthritis.

Enzyme involved in arthritis

Rheumatoid arthritis is a chronic inflammatory disease which causes the join destruction. Cyclooxygenase enzyme causes the increase in prostaglandin synthesis at the infection site.There are particularly two forms of

cyclooxygenase, which are, cyclooxygenase-1 (COX-1) that maintains house-keeping functions and the other one is cyclooxygenase-2 (COX-2), whichshows response towards inflammatory condition. COX-2is reported to be present in synovial tissue of patients with rheumatoid arthritis and to a less extent COX-1 is also present. COX-2 expression in the rheumatoid synovium is induced by proinflammatory cytokines, specially by IL-1, whereas,COX-2 expression is inhibited by corticosteroids[9]. Cyclooxygenase (COX-2) has been shown to be upregulated *in vitro* by inflammatory agents, like lipopolysaccharide, IL-1 and TNF[7]. These mediators are involved in rheumatoid arthritis and cancer-induced angiogenic processes. It is reported thatcyclooxygenase (COX)-2 upregulation in osteoarthritis and rheumatoid arthritis is associated with the pain and inflammation during the diseased state. COX-2 is generally not expressed normally, but is rapidly induced in response to inflammatory stimuli and is responsible for production of large amounts of prostaglandin E2 (PGE2)and other arachidonic acid metabolites at the inflammatory sites.COX-2 is involved in pathophysiologic processes, such as, inflammation, pain, and fever.In the late 1980s, it was shown that expression of COX activity is markedly stimulated by interleukin-1 in fibroblasts and monocytes and gets inhibited by corticosteroids[10].

Molecular docking

Molecular docking method was conducted to identify the phytochemical from the plant extract, that act as a ligand to form a strong covalent bond with the bacterial protein in order to inhibit the microbe. The Discovery studio module of BIOVIA software was used for identifying molecular interaction and perform molecular docking. The sdf files for the phytochemicals present in *Azadirachta indica* plant were downloaded from PubChem website. The protein database code forthe enzyme Cyclooxygenase was identified from the website (rcsb). To carry out the docking procedure, the active site of the enzyme was first identified in the "receptor cavity" protocol under "receptor-ligand interaction" menu. Molecular docking was carried out using the CDocker protocol of BIOVIAsoftware under "receptor-ligand interaction". The enzyme molecule was considered as the receptor in the interaction and the phytochemical was treated as the ligand. The "-CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" were used as indicator to interpret the quality of molecular docking. The high positive value of them indicated a good interaction between the ligand and the receptor. Thus, the interactions with high values indicated the phytochemical showed activity in inhibiting the enzyme associated with the disease.

RESULTS AND DISCUSSION

Figure 1 shows the active site of the cyclooxygenase enzyme. It appears as light green color. CDOCK is a molecular dynamics (MD) simulated-annealing-based algorithm. It is a grid-based molecular docking method which is optimized for accuracy. The ligand conformations were obtained by Molecular Dynamic methods.-CDOCKER energy was calculated based on the internal ligand strain energy and receptor-ligand interaction energy. -CDOCKER interaction signifies the energy of the nonbonded interaction that exists between the protein and the ligand. The criteria for best interaction was chosen based on a) high positive value of -CDOCKER energy and b)small difference between -CDOCKER energy and -CDOCKER interaction energy.

Table 1 shows that Interaction between cyclooxygenase- anthelmintic to be the highest -CDOCKER positive value which is(28.0012) and the minimum difference between –CDOCKER energy and interaction energy is(1.5807).Interaction values for cyclooxygenase-anthelmintic is followed by interaction between cyclooxygenase-ethyl acetate.This shows that anthelmintic and ethyl acetate can effectively interact with cyclooxygenase thereby inhibiting itsenzymatic activity. Whereas, Nimbin and anticarcinogenic phytochemicals cannot detect the enzyme. So key phytochemicals in *Azadirachtaindica*preventing rheumatoid arthritis could be anthelmintic and ethyl acetate.

CONCLUSIONS

It is reported previously that neem (*Azadirachta indica)* plant has medicinal value which can act as curative for many diseases and is also used for rheumatoid arthritis. This study was carried out to provide the theoretical basis of this

observation. Using Discovery studio module of BIOVIA software, molecular docking operation was performed to identify the phytochemical (Anthelmintic, Petroleum ether, Nimbolid, Ethyl acetate, Nimbin, Anticarcinogenic) which can have a significant interaction with the vital enzyme (cyclooxygenase). It was found that Anthelmintic can form strong bond with the enzyme successfully inhibiting the enzyme. But Nimbin, Anticarcinogenic cannot interact with enzyme. Thus, this study shows that the presence of Anthelmintic, Ethyl acetate provides the medicinal value against cyclooxygenase enzyme of rheumatoid arthritis.

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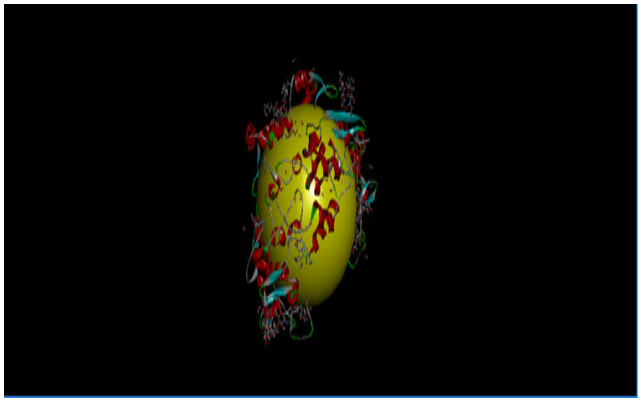

Figure 1. Active site of cyclooxygenase

Table 1. Results of CDocking of phytochemicals with cyclooxygenase (cox2)

SL NO	LIGAND	- C DOCKER ENERGY	- C DOCKER INTERACTION ENERGY	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	Anthelmintic	28.0012	29.5879	1.5807
2	Petroleum ether	16.976	16.3174	-0.6586
3	Nimbolid	-199.875	-32.6648	-235.5398
4	Ethyl acetate	18.103	20.2075	2.1045
5	Nimbin	Failed	Failed	NA
6	Anticarcinogenic	Failed	Failed	NA

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RESEARCH ARTICLE

A Study on the Performance of Some Multi-Response Optimization Methods for Usm Process

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ABSTRACT

Ultrasonic machining (USM) process is use for cutting of non-conductive, brittle workpiece materials such as inorganic glasses, titanium alloys and engineering ceramics etc. Unlike other non-traditional machining processes, it doesnot thermally damage the workpiece or introduce significant levels of residual stress. Ultrasonic machining process has multiple performance measures, e.g. material removal rate (MRR), tool wear rate (TWR), surface roughness (SR) etc, which are affected by several process parameters. In the present study, four multi response optimization methods like Grey Relational Analysis (GRA), Multi Response S/N Ratio (MRSN), Weighted S/N Ratio (WSN) and VIKOR Method are presented and a set of past experimental data on USM process is analysed using these methods. The relative performances of these methods are then compared. The result shows that all the four methods give the same optimal condition for USM process but Weighted S/N ratio (WSN) method is preferred as it requires lesser mathematical calculations compare to others

Keywords: Blend, In Silico, 12α-d-Glucose, Dichloro-Ethylene

INTRODUCTION

Materials play an important role in the advancement of science and technology and the human society. Advancement in automotive, aircraft, electronics industries demand for the requirement of advanced materials. As these are working in adverse conditions, the materials used should have the required properties like high impact strength, high hardness, high temperature resistance, high corrosion resistance, low reactivity, low weight etc. In order to fulfil the demands, the researchers have been working since long to develop new types of materials. The

demand for macro-, micro- and nano products and components of difficult-to-machine materials such as tool steel, carbides, super alloys, titanium alloys and nanostructure materials has been rapidly increasing in automotive, aerospace, electronics, optics, medical devices and communications industries. Conventional machining is incapable of machining such materials with desired accuracy and surface finish. Non-traditional machining processes (like Electrical Discharge Machining (EDM), Electrochemical Machining (ECM), Ultrasonic Machining (USM) etc.) offer a better alternative or sometimes the only alternative in generating accurate 3-D complex shaped features and components of these difficult-to- machine materials. A lot of work has been carried out in the field of process optimization. The researchers have developed a number of optimization techniques to fulfil the current requirements.Caydas*et al.*[1] developed an artificial neural network (ANN) and regression model to predict surface roughness of AA7075 aluminium alloy in abrasive water jet machining (AWJ) process.

The machining parameters like traverse speed, water jet pressure, standoff distance, abrasive grit size and abrasive flow rate were considered as model variables. The statistical analysis showed that the water jet pressure was an utmost parameter on surface roughness. The microstructures of machined surfaces were also studied by scanning electron microscopy (SEM). Rao *et al.*[2] studied the optimization of the surface roughness of die sinking electric discharge machining (EDM) by considering the simultaneous affect of various input parameters. The experiments were carried out on Ti6Al4V, HE15, 15CDV6 and M-250 work pieces. Experiments were conducted by varying the peak current and voltage and the corresponding values of surface roughness (SR) were measured. A hybrid model was developed and optimization of SR in die sinking electric discharge machining was carried out using artificial neural network (ANN) and genetic algorithm (GA). Ramakrishnan and Karunamoorthy[3] developed artificial neural network (ANN) models and multi response optimization technique to predict and select the best cutting parameters of wire electro-discharge machining (WEDM) process.

Experiments were performed under different cutting conditions of pulse on time, delay time, wire feed speed and ignition current to predict the performance characteristics namely, material removal rate and surface roughness. The responses were optimized concurrently using multi response signal-to-noise (MRSN) ratio in addition to Taguchi's parametric design approach. Zain *et al.*[4] proposed an integrated Artificial Neural Network (ANN) and Simulated Annealing (SA) techniques to estimate optimal process parameters in abrasive water jet (AWJ) machining operation. The considered process parameters include traverse speed, water jet pressure, standoff distance, abrasive grit size and abrasive flow rate.

The optimal values of these process parameters were targeted for giving a minimum value of average surface roughness (Ra). Yadav *et al.* [5] proposed an Artificial neural network (ANN) model for electrical discharge diamond cut-off grinding (EDDCG) process, to correlate the input process parameters namely current, pulse-on time, duty factor and wheel speed with the performance measures namely, material removal rate (MRR) while machining cemented carbide. Acherjee*et al.*[6] proposed a hybrid approach based on Taguchi method and artificial neural network (TM-ANN) to improve the effectiveness of optimizing quality characteristics in laser transmission welding process. The input process parameters considered were power, welding speed and focal distance. Vundavilli*et al.*[7] proposed an expert system for abrasive water jet machining (AWJM) process using Fuzzy logic (FL). It was found that the performance of AWJM in terms of depth of cut depends on various process parameters, such as diameter of focusing nozzle, water pressure, abrasive mass flow rate and jet traverse speed.

The developed expert system eliminates the need of extensive experimental work, to select the most influential AWJM parameters on the depth of cut. Joshi andPande [8] worked on intelligent approach for process modeling and optimization of electric discharge machining (EDM). Physics based process modeling using finite element method (FEM) has been integrated with the soft computing techniques like artificial neural networks (ANN) and genetic algorithm (GA) to improve prediction accuracy of the model with less dependency on the experimental data. A two-dimensional axi-symmetric numerical (FEM) model of single spark EDM process has been developed based on more realistic assumptions such as Gaussian distribution of heat flux, time and energy dependent spark radius, etc. to

predict the shape of crater, material removal rate (MRR) and tool wear rate (TWR). Ghosal and Manna [9] investigated on machining of Al/Al_2O_3 MMC by ytterbium fiber laser. The effects of the different parameters on the response characteristics were explained. A comprehensive mathematical models for correlating the interactive and higher-order influences of various machining parameters such as laser power, modulation frequency, gas pressure, wait time, pulse width on the machining performance criteria e.g., metal removal rate and tapering phenomena has been developed for achieving controlled over fiber laser machining process.

The response surface methodology (RSM) was employed to achieve optimum responses i.e., minimum tapering and maximum material removal rate. Sharma and Yadava [10] presented the modeling and optimization of cut quality characteristics during Nd:YAG laser cutting of aluminum alloy thin sheet along the curved profile. The cut quality characteristics considered are average kerf deviation (Da) and average kerf taper (Ta). The essential input process parameters were identified as arc radius of curve profile, oxygen pressure, pulse width, pulse frequency and cutting speed. First, second order response surface model was developed for each Da and Ta using hybrid approach of Taguchi methodology (TM) and response surface methodology (RSM). The effect of input process parameters on each cut quality (Da and Ta) was also studied. Second, preferred operating laser cutting parameters were obtained using grey relational analysis (GRA) with entropy measurement (EM) to minimize Da and Ta together. In the present study a comparison is made between the most widely used multi response optimization techniques like GRA, MRSN, WSN and VIKOR methods and a suitable optimization technique for USM process is proposed for practical realization.

MATERIALS AND METHODS

Taguchi [11, 12] categorized the response variables into three different types, i.e., smaller the better, larger the better and nominal the best. Assuming that there are m experimental trials and in each trial, quality losses of a set of p response variables are measured. Quality loss (L_{ij}) for j*th* response corresponding to$i$*th* trial (i=1, 2,…,m; j=1,2,…,p) for different types of response variables are given as follows:

For smaller the better, $L_{ij} = \left(\frac{1}{n}\sum_{k=1}^{n} y^2_{ijk}\right)$ (1)

For larger the better, $L_{ij} = \left(\frac{1}{n}\sum_{k=1}^{n} \frac{1}{y^2_{ijk}}\right)$(2)

For nominal the best, $L_{ij} = \left(\frac{S_{ij}^2}{\bar{y}_{ij}^2}\right)$(3)

where, $\bar{y}_{ij} = \frac{1}{n}\sum_{k=1}^{n} y_{ijk}$, $S_i^2 = \frac{1}{n-1}\sum_{k=1}^{n}(y_{ijk} - \bar{y}_j)^2$

n represents the number of repeated experiments, y_{ijk} is the experimental value of j*th* response variable in i*th* trial at k*th* replication and L_{ij} is the computed quality loss for j*th* response in i*th* trial.

The Signal-to-Noise ratio value (η_{ij}) is obtained by putting the value of L_{ij} for j*th* response in i*th* trial in the equation:

$\eta_{ij} = -10\log_{10}L_{ij}$(4)

The quality loss (L_{ij}) is normalized to reduce the variability among different responses. The normalized quality loss (S_{ij}) is given as:

$S_{ij} = L_{ij}/L_{i}$(5)

where$L_{i} = \frac{1}{m}\sum_{i=1}^{m} L_{ij}$ is the average quality loss for j*th* response.

Sometimes, signal-to-noise ratio is normalized instead of quality loss and is scaled between 0 and 1.

$Y_{ij} = (\eta_{ij} - \eta_j^{min})/(\eta_j^{max} - \eta_j^{min})$(6)

whereY_{ij} = scaled signal-to-noise ratio value for j*th* response in$i$*th* trial, η_j^{min} = min $\{\eta_{1j}, \eta_{2j},...,\eta_{mj}\}$ and η_j^{max}= max $\{\eta_{1j}, \eta_{2j},...,\eta_{mj}\}$.

The optimal parametric setting in all the four multi-response optimization methods involves:
Step 1: Converting the multiple responses into a single process performance index (PPI) for optimization.
Step 2: Determining the influencing factors and then, obtaining the optimal factor-level combination.
Step3: Validating the optimal factor-level combination using confirmatory experiment.
The four methods (GRA, MRSN ratio, WSN ratio and VIKOR) mainly differ with respect to the first step, i.e., methodology used for converting the multiple responses into the PPI value. The remaining two steps are the same for all the four methods of multi-response optimization.
The steps involve in finding the process performance index (PPI) value for the considered multi-response optimization methods are discussed below [13].

Grey Relational Analysis (GRA) method

In this method, Grey Relational Grade (GRG) is considered as the PPI. The steps for obtaining PPI are as follows:
Step 1: Calculation of the Signal-to-Noise ratio (η_{ij}) values for all the responses for all the trialsusing equation (4).
Step 2: Obtaining the scaled Signal-to-Noise ratio (Y_{ij}) values for all the responses for all the trials using equation (6).
Step 3: Computation of the grey relational coefficients.
Grey relational coefficient (γ_{ij}) for *jth* response in *ith* trial is computed as follows:

$$\gamma_{ij} = (\Delta_j^{min} + \xi\Delta_j^{max})/(\Delta_{ij} + \xi\Delta_j^{max}) \quad (7)$$

where $\Delta_{ij} = | 1- Y_{ij} |$, $\Delta_j^{min} = \min\{\Delta_{1j}, \Delta_{2j},...,\Delta_{mj}\}$, $\Delta_j^{max} = \max\{ \Delta_{1j}, \Delta_{2j},...,\Delta_{mj} \}$
and ξ is the distinguishing coefficient ($\xi \in [0,1]$). The distinguishing coefficient is used to expand or compress the range of grey relational coefficient and is usually taken as 0.5.
Step 4: Calculating the grey relational grade (GRG_i) corresponding to *ith* trial as follows:

$$GRG_i = \sum_{j=1}^{p} W_j \gamma_{ij} \quad (8)$$

whereW_j is the weight for *jth* response and $\sum_{j-1}^{p} W_j = 1$.

Multi response S/N ratio (MRSN) method

In the MRSN ratio method, the MRSN ratio is taken as the PPI value which can be obtained using the following steps:
Step 1: Obtaining the scaled quality loss (S_{ij}) for each response in each trial as follows:

$$S_{ij} = (L_{ij} - L_j^{min})/(L_j^{max} - L_j^{min}) \quad (9)$$

whereS_{ij}= scaled quality loss for *jth* response in *ith* trial, $L_j^{min} = \min\{L_{1j},L_{2j},...,L_{mj}\}$ and $L_j^{max} = \max\{L_{1j}, L_{2j},...,L_{mj}\}$.
Step 2: Computing the total quality loss (TL_i) for the *ith* trial as given below:

$$TL_i = \sum_{j=1}^{p} W_j S_{ij} \quad (10)$$

Step 3: Determining the multi-response SN ratio ($MRSN_i$) for *ith* trial as follows:

$$MRSN_i = -10\log_{10}(TL_i) \quad (11)$$

Weighted S/N ratio (WSN) method

In this method, the WSN ratio is considered as the PPI value. The computational procedure for this method can be described as below:
Step 1: Computing the Signal-to-Noise ratio values for all the responses for all the trials using equation (4).
Step 2: Obtaining the scaled signal-to-noise ratio values for all the responses for all the trials using equation (6).
Step 3: Computing the WSN ratio value for *ith* trial using the following equation:

$$WSN_i = \sum_{j-1}^{p} W_j V_{ij} \quad (12)$$

VIKOR method

Here, the VIKOR index is treated as the PPI value. The VIKOR index is computed using the following five steps:
Step 1: Computing the Signal-to-Noise ratio values for all the responses for all the trials using equation (4).
Step 2: Obtaining the scaled Signal-to-Noise ratio values for all the responses for all the trials using equation (6).
Step 3: Determination of ideal and negative-ideal solutions.

The ideal (A^*) and the negative-ideal (A^-) solutions, which represent the maximum and minimum Signal-to-Noise ratio values of all the experimental trials, are as follows:

$A^* = \{\max Y_{ij} \mid i = 1, 2,...,m\}$

$= \{Y_1^*, Y_2^*,.....Y_P^*\}$ (13)

$A^- = \{\min Y_{ij} \mid i = 1,2,...,m\}$

$= \{Y_1^-, Y_2^-,.....Y_P^-\}$ (14)

Step 4: Calculation of the utility and regret measures for each experimental trial.
The utility and regret measures for *ith* experimental trial, S_i and R_i respectively, can be obtained as follows:

$S_i = \sum_{j=1}^{p} [W_j(Y_j^* - Y_{ij})/(Y_j^* - Y_j^-)]$ (15)

$R_i = \text{Max}_j[W_j(Y_j^* - Y_{ij})/(Y_j^* - Y_j^-)]$ (16)

Step 5: Calculation of the VIKOR index of *ith* experimental trial.
The VIKOR index of *ith* experimental trial, Q_i, can be expressed as follows:

$Q_i = \nu [(S_i - S^*)/(S^- - S^*)] + (1- \nu) [(R_i - R^*)/(R^- - R^*)]$; $i = 1,2,....m$ (17)where $S^*=Min\ S_i$, $S^- = Max\ S_i$, $R^*=Min\ R_i$, $R^-=Max\ R_i$and ν is the weight of the maximum group utility which is usually set to be 0.5 .

EXPERIMENTAL DETAILS

The experimental data was taken from a previous journal "An Experimental Study on Ultrasonic Machining of Pure Titanium using Designed Experiments" by Jatinder Kumar and J.S.Khamba [14]. In their paper, they investigated the machining characteristics, i.e., tool wear rate (TWR) and surface roughness (SR) using pure titanium workpiece. The input parameters considered were tool material, abrasive material, grit size of the slurry used and power rating of the machine. The optimal condition for each machining characteristic was obtained separately using Taguchi method. The limitation of this method is that the optimal condition for multiple machining characteristics cannot be known. In the present work, same data is used for comparison of various multi response optimization techniques like GRA method, MRSN ratio, WSN ratio and VIKOR method. These techniques give the optimal condition for multiple machining characteristics. The input parameters taken were Tool material, Abrasive type, Grit size and Power rating. The output parameters taken were Tool wear rate and Surface roughness. The input parameters and their levels were taken as shown in table 1.

The constant parameters were taken as follows:
Frequency of vibration = 21 KHz
Static load = 1.63 Kg
Amplitude of vibration = 25.3 – 25.8 μm
Depth of cut = 2 mm
Thickness of workpiece = 10 mm
Slurry concentration = 25%
Tool geometry = Straight cylindrical with diameter 8 mm
Slurry temperature = 28 C
Slurry flow rate = 36.4 x 10^3 mm^3/min
Slurry media = water
L_{18} orthogonal array was selected for the given input parameters as shown in the table 2.

The experiments were conducted as per the L_{18} orthogonal array and readings were noted as shown in the table 3. In the present study, these experimental readings have been taken for the calculation purpose in order to compare various multi response optimization techniques like GRA method, MRSN ratio, WSN ratio and VIKOR method.The expressions for quality loss, S/N ratio and Scaled S/N ratio have been discussed in section 2 and the calculated values are shown in table 4.

Grey relational analysis (GRA) method:

In this method, Grey relational grade (GRG) is considered as the process performance index value. The steps to calculate the GRG values have been discussed in chapter 3 and calculated values are shown in table 5.

Multi response S/N ratio (MRSN) method

In this method, the MRSN ratio is taken as the process performance index value. The steps to calculate the MRSN ratio have been discussed in section 2 and calculated values are shown in table 6.

Weighted S/N ratio (WSN) method

In this method, WSN ratio is considered as the process performance index value. The steps required to calculate the WSN ratio have been discussed in section 2 and calculated values are shown in table 7.

VIKOR method

In this method, VIKOR index is considered as the process performance index value. The steps to calculate the VIKOR index have been discussed in section 2 and calculated values are shown in table 8.

Analysis of Variance (ANOVA)

The percentage contribution of various input parameters on the selected machining characteristics can be estimated by performing ANOVA.

Grey Relational Analysis (GRA) method

where SS = Sum of Square

DF = Degree of Freedom = Level – 1

MS = Mean Square = SS / DF

F = F value = (MS due to factor / MS due to error)

Higher the F value of the input parameter means higher effect of that parameter on performance characteristic. In Grey Relational Analysis (GRA) method, greater value of level average means better quality. So, optimal condition using Grey Relational Analysis method is $\mathbf{A_4B_1C_3D_1}$.

Multi response S/N ratio (MRSN) method

In Multi response S/N ratio (MRSN) method, greater value of level average means better quality. So, optimal condition using Multi Response S/N ratio method is $\mathbf{A_4B_1C_3D_1}$.

Weighted S/N ratio (WSN) method

In Weighted S/N ratio (WSN) method, greater value of level average means better quality. So, optimal condition using Weighted S/N ratio method is $\mathbf{A_4B_1C_3D_1}$.

VIKOR method

In VIKOR method, smaller value of level average means better quality. So, optimal condition using VIKOR method is $\mathbf{A_4B_1C_3D_1}$.

RESULTS AND DISCUSSION

The contribution of each input parameter i.e. Tool material (A), Abrasive type (B), Grit size (C) and Power rating (D) on the performance parameters - Tool wear rate (TWR) and Surface roughness (SR) has been calculated using Analysis of variance (ANOVA). In GRA method, it is found that tool material (A) has the highest contribution of 33.84% followed by power rating (D), grit size (C) and abrasive type (B) having contribution of 26.97%, 23.43% and 5.50% respectively. In MRSN method, it is found that tool material (A) has the highest contribution of 32.32% followed by power rating (D), grit size (C) and abrasive type (B) having contribution of 31.96%, 21.06% and 9.28% respectively. In WSN method, it is found that tool material (A) has the highest contribution of 29.97% followed by power rating (D), grit size (C) and abrasive type (B) having contribution of 28.47%, 27.21% and 8.80% respectively. In VIKOR method, it is found that tool material (A) is having the highest contribution of 38.54% followed by power rating (D), abrasive type (B) and grit size (C) having contribution of 26.70%, 10.61% and 10.43% respectively.

The level averages for each input parameter has been calculated for various process performance index (PPI) values. Greater value of level average of GRG, MRSN ratio and WSN ratio signify better quality. On the other hand, smaller value of level average of VIKOR index signifies better quality. In all the four methods, the optimal condition is obtained as $\mathbf{A_4B_1C_3D_1}$, i.e. the optimal combination will be as follows:
Tool material (A) – Ti alloy
Abrasive type (B) – Alumina
Grit size (C) – 500
Power rating (D) – 100 Watt

CONCLUSIONS

i. There are only a few multi response optimization techniques like Grey Relational Analysis (GRA), Multiple Response Signal-to-Noise (MRSN) ratio, Weighted Signal-to-Noise (WSN) ratio and VIKOR method which use simple computational procedures and are therefore very useful for the engineers.
ii. Using the above methods in USM process, it is found that tool material is having the highest influence on the output performance followed by power rating, grit size and abrasive type.
iii. In all the four methods, the optimal combination is obtained as $A_4B_1C_3D_1$, i.e., tool material – Titanium alloy, Abrasive type – Alumina, Grit size – 500 and Power rating – 100 Watt.
iv. All the four methods are found to be suitable for the present study but WSN method is preferred as it involves less calculation compared to other methods.

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Table 1 Input parameters

SYMBOL	PARAMETER	LEVEL 1	LEVEL 2	LEVEL 3	LEVEL 4	LEVEL 5
A	TOOL MATERIAL	HCS	HSS	TITANIUM	TITANIUM ALLOY	CEMENTED CARBIDE
B	ABRASIVE TYPE	ALUMINA	SILICON CARBIDE	BORON CARBIDE		
C	GRIT SIZE	220	320	500		
D	POWER RATING	100	250	400		

Table 2 L_{18} orthogonal array

EXPERIMENT NO.	A	B	C	D
1	1	1	1	1
2	1	2	2	2
3	1	3	3	3
4	2	1	1	2
5	2	2	2	3
6	2	3	3	1
7	3	1	2	1
8	3	2	3	2
9	3	3	1	3
10	4	1	3	3

11	4	2	1	1
12	4	3	2	2
13	5	1	2	3
14	5	2	3	1
15	5	3	1	2
16	1	1	3	2
17	1	2	1	3
18	1	3	2	1

Table 3 Experimental readings

EXPERIMENT NO.	TWR (mg/min)			SR (microns)		
	R1	R2	R3	R1	R2	R3
1	3.87	4.13	3.56	0.85	0.98	0.92
2	4.85	5.28	4.57	1.24	1.18	1.05
3	6.56	6.30	7.00	0.73	0.70	0.52
4	3.20	3.00	3.36	1.17	1.11	0.82
5	8.16	8.08	8.25	1.20	1.19	1.32
6	1.88	1.64	1.97	0.53	0.64	0.60
7	0.57	1.33	0.54	0.68	0.50	0.72
8	1.40	1.89	1.21	0.73	0.89	0.90
9	6.00	6.50	5.77	2.14	2.20	1.90
10	0.95	0.62	0.87	0.56	0.68	0.75
11	0.72	0.72	0.56	0.60	0.79	0.64
12	1.86	1.95	1.78	0.85	0.86	0.81
13	7.75	7.95	8.26	1.04	1.12	0.97
14	5.12	5.06	5.50	0.75	0.65	0.60
15	9.37	9.88	9.10	1.82	1.68	1.70
16	1.45	1.70	1.40	0.77	0.83	0.66
17	12.30	12.00	12.36	2.18	2.29	2.26
18	3.23	2.47	4.00	0.73	0.74	0.92

Table 4 Calculation of Quality loss, S/N ratio and Scaled S/N ratio

TRIAL	FACTOR				QUALITY LOSS (L_{ij})		S/N RATIO (η_{ij})		SCALED S/N RATIO (Y_{ij})	
	A	B	C	D	TWR	SR	TWR	SR	TWR	SR
1	1	1	1	1	14.90	0.84	-11.73	0.76	0.3971	0.6716
2	1	2	2	2	24.09	1.34	-13.82	-1.27	0.3142	0.4961
3	1	3	3	3	43.91	0.43	-16.43	3.66	0.2106	0.9222
4	2	1	1	2	10.18	1.09	-10.08	-0.37	0.4625	0.5739
5	2	2	2	3	66.64	1.53	-18.24	-1.85	0.1388	0.4460
6	2	3	3	1	3.37	0.35	-5.27	4.56	0.6533	1.0000
7	3	1	2	1	0.79	0.41	1.02	3.87	0.9028	0.9404
8	3	2	3	2	2.33	0.71	-3.67	1.49	0.7168	0.7346
9	3	3	1	3	37.18	4.34	-15.70	-6.37	0.2396	0.0553
10	4	1	3	3	0.68	0.45	1.67	3.47	0.9286	0.9058

11	4	2	1	1	0.45	0.46	3.47	3.37	1.0000	0.8971
12	4	3	2	2	3.48	0.71	-5.42	1.49	0.6474	0.7346
13	5	1	2	3	63.83	1.09	-18.05	-0.37	0.1464	0.5739
14	5	2	3	1	27.36	0.45	-14.37	3.47	0.2923	0.9058
15	5	3	1	2	89.41	3.01	-19.51	-4.78	0.0884	0.1927
16	1	1	3	2	2.32	0.57	-3.65	2.44	0.7176	0.8168
17	1	2	1	3	149.35	5.03	-21.74	-7.01	0.0000	0.0000
18	1	3	2	1	10.84	0.64	-10.35	1.94	0.4518	0.7736

Table 5 Calculation of Grey relational coefficient and Grey relational grade

TRIAL	FACTOR				GREY RELATIONAL COEFFICIENT (γ_{ij})		GREY RELATIONAL GRADE (GRG_i)
	A	B	C	D	TWR	SR	
1	1	1	1	1	0.4534	0.6036	0.5285
2	1	2	2	2	0.4216	0.4980	0.4598
3	1	3	3	3	0.3878	0.8654	0.6266
4	2	1	1	2	0.4819	0.5399	0.5109
5	2	2	2	3	0.3673	0.4744	0.4208
6	2	3	3	1	0.5905	1.0000	0.7952
7	3	1	2	1	0.8372	0.8935	0.8654
8	3	2	3	2	0.6384	0.6532	0.6458
9	3	3	1	3	0.3967	0.3461	0.3714
10	4	1	3	3	0.8750	0.8415	0.8582
11	4	2	1	1	1.0000	0.8293	0.9146
12	4	3	2	2	0.5864	0.6532	0.6198
13	5	1	2	3	0.3694	0.5399	0.4546
14	5	2	3	1	0.4140	0.8415	0.6278
15	5	3	1	2	0.3542	0.3825	0.3684
16	1	1	3	2	0.6391	0.7318	0.6854
17	1	2	1	3	0.3333	0.3333	0.3333
18	1	3	2	1	0.4770	0.6883	0.5826

Table 6 Calculation of Scaled quality loss, Total quality loss and MRSN ratio

TRIAL	FACTOR				SCALED QUALITY LOSS (S_{ij})		TOTAL QUALITY LOSS (TL_i)	MRSN RATIO
	A	B	C	D	TWR	SR		
1	1	1	1	1	0.0970	0.1047	0.1008	9.9654
2	1	2	2	2	0.1587	0.2115	0.1851	7.3259
3	1	3	3	3	0.2918	0.0171	0.1544	8.1135
4	2	1	1	2	0.0653	0.1581	0.1117	9.5195
5	2	2	2	3	0.4445	0.2521	0.3483	4.5804
6	2	3	3	1	0.0196	0.0000	0.0098	20.0877
7	3	1	2	1	0.0023	0.0128	0.0076	21.1918
8	3	2	3	2	0.0126	0.0769	0.0448	13.4872
9	3	3	1	3	0.2466	0.8526	0.5496	2.5995
10	4	1	3	3	0.0015	0.0214	0.0114	19.4309
11	4	2	1	1	0.0000	0.0235	0.0118	19.2812

12	4	3	2	2	0.0203	0.0769	0.0486	13.1336
13	5	1	2	3	0.4256	0.1581	0.2918	5.3491
14	5	2	3	1	0.1807	0.0214	0.1010	9.9568
15	5	3	1	2	0.5974	0.5684	0.5829	2.3440
16	1	1	3	2	0.0126	0.0470	0.0298	15.2578
17	1	2	1	3	1.0000	1.0000	1.0000	0.0000
18	1	3	2	1	0.0698	0.0619	0.0658	11.8177

Table 7 Calculation of WSN ratio

TRIAL	FACTOR				WSN RATIO
	A	B	C	D	
1	1	1	1	1	0.5343
2	1	2	2	2	0.4051
3	1	3	3	3	0.5664
4	2	1	1	2	0.5182
5	2	2	2	3	0.2924
6	2	3	3	1	0.8266
7	3	1	2	1	0.9216
8	3	2	3	2	0.7257
9	3	3	1	3	0.1474
10	4	1	3	3	0.9172
11	4	2	1	1	0.9485
12	4	3	2	2	0.6910
13	5	1	2	3	0.3601
14	5	2	3	1	0.5990
15	5	3	1	2	0.1405
16	1	1	3	2	0.7672
17	1	2	1	3	0.0000
18	1	3	2	1	0.6127

Table 8 Calculation of Utility measure, Regret measure and VIKOR index

TRIAL	FACTOR				UTILITY MEASURE (S_i)	REGRET MEASURE (R_i)	VIKOR INDEX (Q_i)
	A	B	C	D			
1	1	1	1	1	0.4656	0.3014	0.4990
2	1	2	2	2	0.5948	0.3429	0.6130
3	1	3	3	3	0.4336	0.3947	0.5851
4	2	1	1	2	0.4817	0.2687	0.4714
5	2	2	2	3	0.7076	0.4306	0.7693
6	2	3	3	1	0.1733	0.1733	0.2035
7	3	1	2	1	0.0784	0.0486	0.0158
8	3	2	3	2	0.2743	0.1416	0.2218
9	3	3	1	3	0.8525	0.4723	0.8916
10	4	1	3	3	0.0828	0.0471	0.0165
11	4	2	1	1	0.0514	0.0514	0.0047
12	4	3	2	2	0.3090	0.1763	0.2784
13	5	1	2	3	0.6398	0.4268	0.7293
14	5	2	3	1	0.4009	0.3538	0.5228

15	5	3	1	2	0.8594	0.4558	0.8771
16	1	1	3	2	0.2328	0.1412	0.1995
17	1	2	1	3	1.0000	0.5000	1.0000
18	1	3	2	1	0.3873	0.2741	0.4276

Table 9 Process Performance Index (PPI) values

TRIAL	PROCESS PERFORMANCE INDEX (PPI)			
	GRG	MRSN RATIO	WSN RATIO	VIKOR INDEX
1	0.5285	9.9654	0.5343	0.4990
2	0.4598	7.3259	0.4051	0.6130
3	0.6266	8.1135	0.5664	0.5851
4	0.5109	9.5195	0.5182	0.4714
5	0.4208	4.5804	0.2924	0.7693
6	0.7952	20.0877	0.8266	0.2035
7	0.8654	21.1918	0.9216	0.0158
8	0.6458	13.4872	0.7257	0.2218
9	0.3714	2.5995	0.1474	0.8916
10	0.8582	19.4309	0.9172	0.0165
11	0.9146	19.2812	0.9485	0.0047
12	0.6198	13.1336	0.6910	0.2784
13	0.4546	5.3491	0.3601	0.7293
14	0.6278	9.9568	0.5990	0.5228
15	0.3684	2.3440	0.1405	0.8771
16	0.6854	15.2578	0.7672	0.1995
17	0.3333	0.0000	0.0000	1.0000
18	0.5826	11.8177	0.6127	0.4276

Table 10 ANOVA results on GRG values

SOURCE	GRG				
	SS	DF	MS	F	% CONTRIBUTION
A	0.1853	4	0.0463	5.78	33.84
B	0.0301	2	0.0150	1.87	5.50
C	0.1283	2	0.0642	8.02	23.43
D	0.1477	2	0.0738	9.22	26.97
ERROR	0.0562	7	0.0080	-	10.26
TOTAL	0.5476	17			100

Table 11 Level averages of GRG values

FACTOR	GRG				
	LEVEL1	LEVEL2	LEVEL3	LEVEL4	LEVEL5
A	0.5360	0.5756	0.6275	**0.7975**	0.4836
B	**0.6505**	0.5670	0.5607	-	-
C	0.5045	0.5672	**0.7065**	-	-
D	**0.7190**	0.5484	0.5108	-	-

Table 12 ANOVA results on MRSN values

SOURCE	MRSN				
	SS	DF	MS	F	% CONTRIBUTION
A	232.8105	4	58.2026	10.52	32.32
B	66.8845	2	33.4422	6.05	9.28
C	151.6930	2	75.8465	13.71	21.06
D	230.2163	2	115.1082	20.81	31.96
ERROR	38.7146	7	5.5306	-	5.37
TOTAL	720.3189	17			100

Table 13 Level averages of MRSN values

FACTOR	MRSN				
	LEVEL1	LEVEL2	LEVEL3	LEVEL4	LEVEL5
A	8.7467	11.3958	12.4262	**17.2819**	5.8833
B	**13.4524**	9.1052	9.6827	-	-
C	7.2849	10.5664	**14.3889**	-	-
D	**15.3834**	10.1780	6.6789	-	-

Table 14 ANOVA results on WSN values

SOURCE	WSN				
	SS	DF	MS	F	% CONTRIBUTION
A	0.4104	4	0.1026	9.50	29.97
B	0.1205	2	0.0602	5.57	8.80
C	0.3725	2	0.1862	17.24	27.21
D	0.3898	2	0.1949	18.05	28.47
ERROR	0.0759	7	0.0108	-	5.54
TOTAL	1.3691	17			100

Table 15 Level average of WSN values

FACTOR	WSN				
	LEVEL1	LEVEL2	LEVEL3	LEVEL4	LEVEL5
A	0.4809	0.5457	0.5982	**0.8522**	0.3665
B	**0.6698**	0.4951	0.4974	-	-
C	0.3814	0.5472	**0.7336**	-	-
D	**0.7404**	0.5413	0.3806	-	-

Table 16 ANOVA results on VIKOR index values

SOURCE	VIKOR index				
	SS	DF	MS	F	% CONTRIBUTION
A	0.6514	4	0.1628	4.93	38.54
B	0.1794	2	0.0897	2.72	10.61
C	0.1764	2	0.0882	2.67	10.43
D	0.4512	2	0.2256	6.83	26.70
ERROR	0.2314	7	0.0330	-	13.69
TOTAL	1.6898	17			100

Table 17 Level averages of VIKOR index values

FACTOR	VIKOR index				
	LEVEL1	**LEVEL2**	**LEVEL3**	**LEVEL4**	**LEVEL5**
A	0.5540	0.4814	0.3764	**0.0998**	0.7097
B	**0.3219**	0.5219	0.5438	-	-
C	0.4695	0.4722	**0.2915**	-	-
D	**0.2789**	0.4435	0.6653	-	-

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RESEARCH ARTICLE

A Survey on Friction Stir Welding for Soft Materials

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ABSTRACT

Friction Stir Welding is a solid state welding process which is used to join the soft materials like aluminium, copper, nickel, titanium etc. It uses heat generated from friction produced by rotating tool and high axial force. At elevated temperature material. Under goes plastic deformation zone which is stirred by rotating tool. On cooling, a solid bond is formed; it is called as weld nugget. FSW Process is characterized by different welding parameters like Rotation Speed, Traverse Speed, Axial load, Tool Geometry which enhances different mechanical properties such as tensile strength, yield strength, hardness, corrosion resistance etc. This paper shows effect of various welding parameters on the characteristics of weld formed during FSW.

Keywords: Friction Stir Welding, Welding nugget, High Speed Steel, Solid State Welding.

INTRODUCTION

During a friction stir welding (FSW) process, a tool rotates while at the same time its pin traverses along the welding direction under a vertical force Mishra and Ma [1]. The process produces inevitably a frictional heat thus softening the material underneath the tool. In order to obtain sufficient frictional heat, the pin length should be of a specified length. For example, Bahrami et al. [2] have welded 6mm thick 7075 aluminum alloy sheets using a pin length of 5.7 mm. Marzbanrad et al. [3] welded 3mm thick 5083 aluminum alloy sheets using a pin with a length of 2.8 mm. Welded 5mm thick pure copper using a pin with a length of 4.7 mm. In general, the pin length is consistently shorter than the thickness of sheets. As a result, the so-called kissing bond is inevitably created in the root of weld. Oosterkamp et al. [4] suggested that the kissing bond represents a partial remainder of the un-welded original butting interface, induced by an insufficient sinking of the pin during the welding process. Rotating tool serves two main functions 1.Heat can be produced by large axial force and high RPM required to soften metal 2.Stirring of materials to form weld nugget by making solid bond on cooling. During the process, material undergoes in a plastic deformation phase at high temperature which forms fine and equaxed recrystallized grains. Due to fine and

recrystallization grains mechanical properties such as tensile strength, yield strength, hardness, elongation etc can be improved (Fig. 1)

Benefits of friction stir Welding

- It can be used with conventional vertical milling machine.
- It utilizes simple, non-consumable and economical tooling.
- No filler material or shielding gas is required to join the material.
- As the soft material used for joining, less energy required to weld.
- No special purpose and costly fixture is required for holding the work piece.

During the process observed zones are as shown in fig.2.,

Heat Affected Zone (HAF): This zone experiences a thermal cycle, but does not undergo any plastic deformation. It retains the same grain structure as the parent material

Weld Nugget (WN): It is the metal structure formed after cooling of stirred zone which creates strong bond between the two metals under the welding. Recrystallized fine grain structures in the form of onion rings are observed.

Thermo-Mechanically Affected Zone (TMAZ): It is highly deformed zone. The base metal contains elongated grains were deformed in an upward flowing pattern around the nugget zone. Although the TMAZ underwent plastic deformation, recrystallization did not occur in this zone due to insufficient deformation strain.

Base Material (BM): The unaffected zone which does not experience effect of welding parameters.

Literature Review

Wei et al.[5] conducted experiments on 2mm thick 01420 Al-Li alloy plates with different welding parameters pin rotation, welding speed, welding pressure. Groove type defect was observed at low speed welding. At very high speed surface quality became poor; groove type defect could be seen. At inappropriate speed, tunnel type defect could be observed. At high axial pressure, it would be caused depression and wavy burrs.

At low axial pressure tunnel and groove type defect occurred. At small shoulder value frictional heat input was low.

It was found that hardness value was high in stir zone than base metal. Hardness tended to decrease with an increase

in heat input due to different thermal effects with welding conditions. Very fine equi axed recrystallized grain structure was obtained in stir zone after dynamic recryastalization. Heat input had little influence on joint strength.

Zhang et al. [6] carried experiments in underwater conditions of AA2219 alloy. Tensile strength of the joint was found to be improved from axial load of 324 MPa by external water cooling action in normal to 341 MPa with deterioration of plasticity of weld nugget. Underwater joint was found to be fractured at the interface between NZ and TMAZ on advancing side during tensile test. Underwater FSW joint exhibits lower hardness in NZ and Higher Hardness in TMAZ and HAZ when compared with normal FSW

Patil et al. [7] investigated effects of different welding speed and tool pin profiles on the weld quality of AA6082-O aluminium where tool rotation was kept constant. Joint fabricated with taper screw thread pin exhibits superior tensile strength than tri-flute pin irrespective of welding speed. Taper screw thread joints fabricated at weld speed of 70 mm/min shows more ultimate and yield strength than weld speed at 60 mm/min and 75 mm/min. Four flute joints fabricated at a welding speed of 60mm/min shows superior properties than 70 mm/min or 85 mm/min Koilraj et al. [8] carried out joining of dissimilar Al-cu alloy AA2219-T87 and Al-Mg alloy AA5083-H321 with taguchi L16 orthogonal design of experiments. He found that fusion welding of dissimilar aluminium alloys was very challenging due to formation of low melting eutectic by constituent element resulting in cracking. Significant drop in hardness from AA2219 unaffected base material to weld nugget on advancing side have been observed. On retreating side only slight drop in hardness was observed from weld nugget AA5083 unaffected base material. In tensile test three weld specimens failed in AA5083 side HAZ. High strength joint can beobtained by placing base material on advancing side. Cylindrical threaded tool profile found to be best during welding. D/d ratio played an important role and contributes to 60 % to the weld strength. Tutar et al. [9]conducted study on non heat treatable

AA3003-H12 aluminum alloy sheets to find optimum welding conditions using taguchi orthogonal array with due Consideration of tensile shear load. Three different parameters rotational speed, plunge depth and dwell time were considered during the study. Plunge depth was found to be the most significant parameter with contribution of 69.26 %.As plunge depth was increased; tensile shear load of fsw joint also increased with expansion of HAZ, TMAZ and SN zones. All fractures of the joints in tensile testing occurred in SZ, where bonding section size was small.
Hardness in SZ decreased as the tensile shear load increased. Fine grain structure in the SZ was found at higher Hardness value.

Kumar et al. [10] investigated effect of rotational speed, weld speed, axial load, on tensile strength and % elongation during welding of dissimilar aluminium AA5083-O and 6061-T6. Study revealed that increase in RPM, axial load and welds speed increases tensile strength up to a point further increase in rpm, axial load and weld speed decreased the tensile strength. It was observed that increase in tool rotation and axial force resulted in increase in percentage elongation whereas increase in welding speed resulted in decrease of percentage elongation.

Kadaganchi et al.[11] formulated a mathematical model with spindle speed, welding speed, and tilt angle and tool geometry to predict the yield strength, tensile strength, % elongation of friction stir welds of AA2014-T6 aluminium alloy. Hexagonal tool profile produces higher pulsating effect and smooth material flow which resulted in improved mechanical properties, whereas conical tool profile produced the lowest mechanical properties. Increase in tool tilt angle led to better consolidation of material which improved mechanical properties. When welding parameters were not appropriate defects like turbulence, warm hole, tunnel effect, crack, excess flash and thinning of weld were observed. Flat faced tools produced pulsating effect and better plastic flow. Welding defects can be eliminated by increasing tool tilt angle

Barekatain et al. [12] studied joining of AA 1050 aluminium alloy and commercially pure copper. The annealed and severely plastic deformed sheets were subjected to friction stir welding (FSW) at different rotation and traverse speeds. It was observed that traverse speed range of 50-100 mm/min and rotation speeds of more than 900 r/min produce welds with appropriate surface in annealed sample. Rotation speed of more than 1000 r/min produces welds with appropriate surface in CGPed (Constrained GroovePressing) samples. This may result from higher strength of CGPed that required higher heat input. The average grain size in the stir zone is finer than that in the base metal. This grain refinement during FSW process leads to greater hardness in the stir zone in comparison with hardness of Al base metal. Several forms of intermetallic compounds are found in weld zone of FSWed annealed and CGPed samples. These compounds mainly consist of Al2Cu and Al4Cu9 Dhancholia et al. [13] examined welding of AA 6061 and AA 7039Aluminum alloys. Welding speed and Rotational speed parameters are varied for the study whereas tensile strength, yield strength, hardness were measured.

Theweld produces at low speed have good mechanical properties than the weld produces at higher speed. The mechanical properties increase with the rotational speed and welding speed but up to a certain level then they start decreasing. Multi objective optimization using Response Surface Methodology (RSM) is used to optimize the friction stir welding parameters to obtain the optimum ultimate tensile strength, yield strength, hardness value and impact strength of dissimilar friction stir welded joint at 95% confidence level Palanivel et al. [14] studied effect of welding speed on mechanical and metallurgical properties of dissimilar welding of AA5083-H111 and AA6351-T6 aluminium alloys. Three kinds of microstructures have been observed, namely unmixed region, mechanically mixed region and mixed flow region. The fracture mode was observed to be a ductile fibrous fracture. In general; FSW at higher welding speeds results in a short exposure time in the weld area with insufficient heat and poor plastic flow of the metal and causes some voids like defects in the joint

CONCLUSIONS

In this paper a study of friction stir welding process has been done. It is revealed that FSW can be used to weld soft materials like aluminium, copper, nickel; titanium etc. successfully.FSW is significantly affected by various welding parameters like rotation speed, weld speed, axial load, and tool geometry etc. Table.1. shows summary of literature review of FSW process being applied to the soft materials. Based on review following conclusions has been drawn-. Hardness in weld zone is higher than heat affected zone due to the recrystallization of grains in weld zone. Ratio of shoulder diameter to pin diameter (D/d) plays an important role and contributes to the strength of weld. Increase in tool rotation and axial force resulted in increase in percentage elongation whereas increase in welding speed resulted in decrease of percentage elongation. Increase in rotational speed (RPM), Weld speed and axial load increases tensile strength up to a point further increase in rotational speed (RPM), Weld speed and axial load decreases the tensile strength. Water media reduces residual stresses in the nugget zone as compared to the normal FSW

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Authors	Material	Tool material	Tool geometry	Welding parameters	Remark
Wei *et al*	01420 Al-Li alloy	1Cr18Ni9Ti	Flat shoulder, Frustum Shape	RPM, Weld Speed, Weld Pressure	Hardness value was high in stir zone than base metal. Hardness tends to decrease with an increase in heat input due to different thermal effects with welding conditions
Zhang *et al*	AA2219-T6	W6Mo5Cr4V2	Conical right hand screwed pin	RPM, Weld Speed, Axial load	Underwater FSW joint exhibits lower hardness in NZ and Higher Hardness in TMAZ and HAZ when compared with normal FSW
Patil *et al*	AA6082-O	0.3Si2C0.3Mn12.1C	Triflute and Taper Screw threaded pin	Weld speed, Tool Pin Profile	Joints with taper screw thread pin exhibits superior tensile strength than tri-flute pin irrespective of welding speed
Koilraj *et al*	AA2219-T87, AA5083-H321	H13 with hardness 55VHN	Straight,Tapered,Threaded	RPM, Weld Speed, Pin Geometry, D/d	Cylindrical threaded tool profile found to be best during welding. D/d ratio played an important role and contributes to 60 % to the weld strength
Tutar *et al*	AA3003-H12	H13 hot work tool steel	Threaded Cylindrical Pin	Plunge depth, Dwell time, RPM	As plunge depth was increased; tensile shear load of fsw joint also increased with expansion of HAZ, TMAZ and SZ zones
Kumar *et al*	AA5083-O and AA6061-T6	-	Cylindrical	RPM, Weld Speed, Axial Force	Increase in RPM, axial load and welds speed increases tensile strength upto a point further decreases the tensile strength. Increase in tool rotation and axial force resulted in increase in percentage elongation whereas increase in welding speed resulted in decrease of percentage elongation.

Kadaganchi et al	AA2014-T6	H13 tool steel	Conical, Triangular, Square, Pentagonal, Hexagonal	RPM, Weld Speed, Tilt angle, Tool Pin Profile	Hexagonal tool profile produces higher pulsating effect and smooth material flow which resulted in improved mechanical Properties, whereas conical tool profile produced the lowest mechanical properties.
Barekatain et.al	AA 1050	H13 tool steel	Cylindrical	RPM, Weld Speed	Welding heat input caused grain growth and decrease in hardness value at Al side of the stir zone. It was found that, generally the weakest parts of weld joints of annealed and CGPed samples were Al base metal and stir zone, respectively. Further investigations showed that several forms of intermetallic compounds were produced.
Dhancholia et.al	AA 6061 and AA 7039	HSS tool	Cylindrical	RPM, Weld Speed	The weld produces at low speed have good mechanical properties than the weld produces at higherspeed. The mechanical properties increase with the rotational speedand welding speed but up to acertain level then they starts decreasing.
Palanivel et al	AA5083-H111, AA6351-T6	high carbon and high chromium steel (HCHCr) oil hardened	Straight square (SS) pin profile	Weld speed, RPM is constant	Lower welding speeds causeimproperconsolidation of material, which leads to the reduction in UTS owing to the defect. The stirring becomes insufficient at higher welding speeds. The material present in the advancing side of the tool does not travel enough to the retreating side, which causes adefect. The tendency of the tool to drag at higher welding speeds also contributes to the lowerUTS.

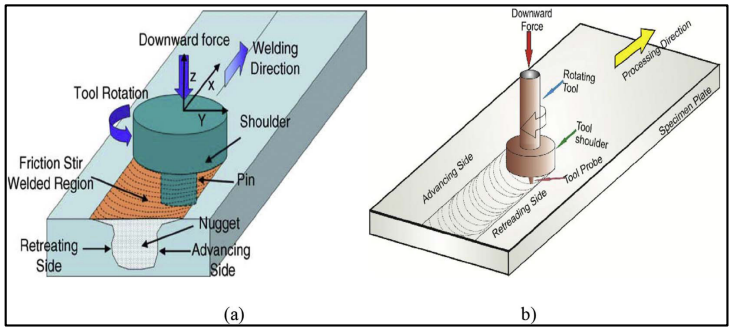

Fig. 1 properties such as tensile strength, yield strength, hardness, elongation etc can be improved

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RESEARCH ARTICLE

Impact of Inflation on Major Financial Ratios

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ABSTRACT

Price remains constant over a period of time and fluctuates due to various reasons. The price floatation cause two types of economic conditions, one is Inflation and another is Deflation. Inflation may well be demarcated as increase in the general price level involve in the influences of production whereas deflation causes fall in the general price level. This study investigates the impact of inflation accounting application on companies' financial performance and financial position by analyzing financial ratios. The financial statements of 42 manufacturing companies covering 7 industrial sectors have been restated in current purchasing power for a period of 5 years (2004-05 to 2008-09). The ratios were calculated on both historical and adjusted numbers of financial statements to form two sets of ratios. In this study the Current Purchasing Power method, financial ratio analysis and different statistical tools like descriptive statistics and t-test have been employed to study the impact of inflation on major financial ratios. This study derived valuable information and results showed that with the impact of inflation, there is significant difference in liquidity, profitability and activity ratios.

Keywords: Manufacturing Firms, Financial Ratios, Inflation, descriptive Statistics, t-test

INTRODUCTION

Inflation continues to be an important reality of economic life in almost all countries. High inflation rates have seriously wind-swept monetary standards in these countries over the past few decades, and have brought forth new patterns of economic behavior. Despite of that, the effects of inflation on the financial performance of economic units go unrecognized in published financial statements. The primary purpose of the financial statements of a company is to give a true and fair picture of financial performance (i.e. profit or loss) of the company for a particular period and financial position (assets and liabilities) of the company for a particular point of time. Those transactions, which can be measured in terms of money, are taken into consideration for recording in the books of account. Money

Measurement Concept is a basic characteristic of accounting.

As per this accounting concept, only those business transactions which are capable of being expressed in terms of money are open for recording by the accounting system. It is also assumed that monetary unit, recording the business transactions, is stable in nature. However, price does not remain constant over a period of time. They tend to change due to various economic, social, political factors. Changes in the price level cause two types of economic conditions, one is Inflation and the other is Deflation. Inflation may be defined as period of general increase in the price level, whereas deflation causes fall in it. These changes in the price level lead to inaccurate presentation of financial statements which otherwise are prepared to present true and fair view of the company's financial health. Another point to consider for preparing the financial statements is the historical cost. In India the financial statements used to present according to actual and cost concept. But this Historical Cost Concept is based on the assumption that the unit of account, i.e. rupee has static value. Moreover, the purchasing power used to change by the passage of time and in India the purchasing power of the rupee is changing and it's rising continuously.

THE RESEARCH PROBLEM

In the past few years of high inflation, companies have reported very high profits on the one hand but on the other, they have faced real financial difficulties. This is so because in reality dividend and taxes have been paid out of capital due to overstated profits arrived by adopting the historical cost concept. This overstatement of profits can have several further effects. When these reported profits are used as the basis of corporate taxes to the Government, it leads to larger tax payments, and the Government becomes an important beneficiary of inflation. Furthermore, if reported profits are used as a basis of corporate decision making, the companies may not be setting prices sufficiently high to ensure an adequate rate of return on a long-term basis, if they have some scope for pricing policies. In addition, dividends are paid out to an excessive degree and thereby they have inadequate level of internal reserves to maintain their real resources intact.

The effect of inflation on the interpretative value of financial statements is much pronounced and it is more frequently put forward as an argument in favour of devaluation from the existing historical cost accounting' system. There are two important aspects of this problem worth monitoring. Firstly, during the period of prolonged inflation various items of the balance sheet, based on different levels of costs and prices, are not comparable in any real sense. In the Profits and Loss account, inventory profits and capital gains get inextricably mixed with operating profit thus making the proper assessment of the earning capacity of the firm difficult, if not impossible. In nutshell, the financial statements become difficult to interpret and their use as a tool of managerial decision-making is much lessened. Secondly, such financial statements mislead the shareholders and other users. The concept of 'profit' and 'maintenance of capital' based on the monetary postulates make the shareholders believe that so long as their money capital is maintained, their interest in the company are fully protected. This belief is, however, erroneous and quite misleading. The real interest of shareholders lies in the yield from business as a going concern and in the eventuality of its winding up in its actual break-up value as opposed to apparent book value. As a consequence of these interpretative difficulties, shareholders and other investors are not provided with information, which enables them to interpret the operating results and to judge the relative effect of price level changes upon a particular enterprise. Such inability arising due to interpretative difficulties of historical cost accounting to properly assess the business position may result in lost business opportunities.

Traditionally, historical cost based accounting information about the operations of companies has ignored the effects of inflation. But the users of financial information, such as current and potential investors, creditors, lenders, suppliers, customers, employees, government authorities and public, need relevant and reliable information about the financial position, performance and changes in the financial position of firms for making economic decisions. Inflation, on the other hand, distorts financial information by creating an impact on the firm's operational and financial results. In a hyperinflationary economy, reporting of operating results and financial position without

restatement is misleading and thus is not useful (International Accounting Standards 29, code 2). Therefore, it is necessary that financial statements reflect the true picture and are free from the negative effects of inflation. Even though inflation accounting has long been debated, a necessary attention is avoided to provide its effects on financial statements of businesses. Hence, this study is conducted to present empirical evidence on the results of inflation on financial statements through analysis of some major ratios. For the purpose, 10 ratios categorized under three groups are analyzed.

LITERATURE REVIEW

Gupta Ramesh and Bhandari L C (1978), in their working paper mention that the whether accountants should be required to adjust reported income for inflation. The objective of this article is to measure the impact of inflation on reported profits and relevant financial ratios. The earnings of 57 companies covering 9 industries have been restated for a period of 7 years (1970-1976). The results emphasize the differential effects on companies with varying inflation rates with general price level adjustments and the significance of monetary gains and losses. The effects of restatement on dividend coverage and tax burden have been suitably highlighted. D. J. Daly (1982), in the article "Inflation, Inflation Accounting and its Effect, Canadian Manufacturing, 1966-82", provides estimates of the effects of inflation in Canada on the reported rate of return in manufacturing firms from 1966 to 1982. It provides estimates for several different concepts of rate of return (both for all assets, whether financed by equity or debt, and for the narrower equity to the owners) and for both a narrow and wide range of financial assets. Comparisons are made with similar studies for the United Kingdom.

Shalom Hochman andOdedPalmon (1985) in their article "The Impact of inflation on the Aggregate Debt-Asset Ratio" demonstrate the impact of inflation on the aggregate debt-asset ratio cannot be determined theoretically. However, it is shown that inflation is likely to increase this ratio when personal income tax schedules are indexed to the price level and/or when leverage-related costs are relatively high and the personal tax rate on income from holding common stocks is relatively low. Whittington G., Saporta V andAjit Singh (1997), in their working paper"The Effects of Hyper-Inflation on Accounting Ratios Financing Corporate Growth in Industrial Economies" described the hyper-inflation can have a severe distortionary effect of the pattern of corporate finance which is apparent from company accounts. A simple algorithm, based upon the method of inflation accounting applied in Brazil, is developed and applied to the accounts of Turkish listed companies for the period 1982-90. The adjusted figures give a more plausible picture of corporate profitability and growth, and this suggests that the adjustment method is substantially successful.

Ambrish Gupta (2000), in his research entitled to "Inflation Accounting- The Indian Context", this study was a modest effort towards a systematic and comprehensive analysis of various aspects for inflation accounting and looks for offering an acceptable solution to this problem in the Indian context. It also made an assessment of the its effect of inflation on the profitability plus financial position, respectively, of the corporate entities, in addition to above it attempt to make an overall review of the financial statements, through ratio analysis and funds flow analysis, in the light of inflation. This study moreover reflects effects of inflation, over sixteen years between 1983-84 to 1998-99, on the financial health of Oil India Ltd. Karapinar A. andZaif F., (2005), in their article "EnflasyonMuhasebesininFinansalTablolarAnalizineEtkisi, (The Effect of Inflation Accounting on Financial Statement Analysis)" In their study, Karapinar and Zaif examined the effects of inflation on accounting practice of companies' financial ratios. Their sample covered the 73 non-financial companies listed Istanbul Stock Exchange as of 2003. The ratios were calculated on both historical and adjusted numbers of financial statements to form two sets of ratios. Results showed that there was no significant change in liquidity, financial, profitability and activity ratios except fixed asset turnover ratios.Akdoğan, Aktas and Unal, in their study in 2009, extended the number of companies in the sample of Karapınar and Zaif. The results covering 146 companies were consistent with the findings of Karapınar and Zaif's study. Their results revealed that a statistically significant change for the whole sample occurs only on Total Assets Turnover. Other ratios did not show any considerable difference.

Charles N'cho-Oguee, Daniel L. Blakley, L.William Murray, andMarolee Beaumont Smith (2011), in their article "Econometric Analysis of Functional Relationship between Inflation and Growth of Firms in South Africa: Empirical Research Findings" this research is to investigate the impact inflation and other factors on the growth of business firms operating in South Africa. Data sets of South African firms' financial statements over the period of 1983-1990 were assembled to permit a detailed examination of the impact of inflation on firm's financial ratios. It has concluded that firm's debt-to-equity, sales-to-assets, and profitability ratios are all positively associated with growth and adversely affected by high inflation; a firm's working capital-to-sales ratio is negatively related to growth and is positively affected by high inflation; and there is a real, measurable impact of the financial instabilities associated with apartheid on firm's growth. Aydın Karapinar, FigenZaifandRıdvanBayirli (2012), this study investigates the impact of inflation accounting application on key financial ratios. These studies related to the financial statements of 132 companies listed in the Istanbul Stock Exchange (ISE) are studied. An analysis of paired samples t test has been conducted on the financial ratios of the companies. The results showed that a significant difference between adjusted cost based financial ratios and historical cost based financial ratios occurs only for current, ratios, equity ratios and noncurrent turnover ratios. The study offered valuable information as to analyzing companies operating in hyperinflation economies. In India serious thinking on having to adjust historical cost accounts to price level change has been rather few and far between.

Patjoshi (2013),in the study investigated the comparison between reported and inflated financial ratios. Financial statements of 42 manufacturing companies covering 7 industrial sectors have been restated in current purchasing power for a period of 5 years (2004-05 to 2008-09). The ratios were calculated on both historical and adjusted financial statements to form two sets of ratios.Similarly, by considering the above data Patjoshi (2013) studied impact of inflation on reported financial performance: of Indian corporate sector,Patjoshi, (2013) examinedthe effect of inflation on measures of financial performance on Indian manufacturing industry, Patjoshi (2013) scrutinized impact of inflation on gross value added and net value added,Patjoshi (2014) observedimpact of inflation on corporate profitability and also Patjoshi (2016) observedimpact of inflation on major stakeholders. All the above studies used the Current Purchasing Power method and different tools of financial statement analysis like comparative and common-size statement analysis.

OBJECTIVES OF THE STUDY

The objectives of the proposed study are to find the impact of inflation on financial performance &position through analyzing the major financial ratios. The objectives of the proposed study are

a) To study the impact of inflation on short term solvency of sample companies through liquidity ratios.
b) To analysis the impact of inflation on financial performance of sample companies through profitability ratios.
c) To find out the impact of inflation on efficiency of resources employed by the sample companies through activity ratios.

HYPOTHESES FOR THE STUDY

To study the research problems and to attain the research objectives, three hypotheses have framed. Broadly, we have attempted to test the null hypothesis against the alternative hypothesis. The null hypothesis and the alternative hypothesis framed for the purpose are:

1. There is no significant difference in between reported and inflated liquidity ratios.
2. There is no significant difference in between reported and inflated profitability ratios.
3. There is no significant difference in between reported and inflated activity ratios.

METHODOLOGY AND TESTS USED IN THE STUDY

The work conducted is a study of 42 undertakings, selected randomly from manufacturing sectors operating in India. The companies so selected are capital intensive, where there is a heavy investment in fixed assets and inventories, profitable and following the same accounting practices throughout the period of study. These sample companies belong to different sectors, viz. Auto, Cement, Chemical, Fertilizer, Food, Petroleum and Steel.

The year-end financial statements of sample companies were used for the comparing the reported and inflated performances. The published annual reports, books, journals, web pages, etc. of the selected companies form the main sources of information. The data so collected are analyzed with the help Current Purchasing Power Method (CPP), Financial Statement Analysis (FSA) and Statistical tools such as; Average, Variance Standard Deviation, Kurtosis, Skewness, and t-test are employed too to draw meaningful conclusion. The t-test is used to compare the values of the means from two groups. The two sample of t-test has been performed because the variances of two groups are assumed to be unequal.

Current Purchasing Power Method

Current Purchasing Power Method of accounting requires the companies to maintain the financial statements on conventional historical cost basis, but it further requires presentation of supplementary statements in items of current purchasing power of currency at the end of the accounting period. In this method the various items of financial statements, i.e. balance sheet and profit and loss account are adjusted with the help of recognized general price index. The consumer price index or the wholesale price index prepared by the Reserve Bank of India can be taken for conversion of historical costs. However, WPI (All Commodities) is being used in this study,

Conversion Process

For analyzing the impact inflation on financial performance the Historical Cost Based (HCB) accounting, financial statements for all the years from 2004-05 to 2008-09 were converted into Accounting for Current Purchasing Power (CPP) financial statements in terms of the index number prevailing in the month of March 2009. The adjustments for inflation are based on movements in wholesale price indexhas presented in Table-1.
Source: Handbook of Statistics on Indian Economics: RBI, 2008-09 Sept15 2009, Office of Economic Advisor Ministry of Commerce and Industry.

The conversion process is explained hereunder

(a) All items of Profit &Loss Account, except Inventory Cost, Depreciation, Taxation, and Equity Dividend have been restated with reference to the "average price index of the year/period" as applicable to the individual year.
(b) Inventory cost has been restated after segregating opening balance of inventories, purchases of raw materials and closing balance of inventories as follows:
- Opening balance of inventories restated in previous year average price index.
- Closing inventories and purchases of raw materials restated in average year price index as applicable to the individual year.

(c) Fixed Assets and Depreciation cost of all the years of study has been adjusted to year base year 2000-01 at year end price index.
(d) Taxation, Dividend on equity shares have been restated with reference to the "end of the year/period index" as applicable to the individual year
(e) The CPP Method divides the Balance Sheet items into two categories: Monetary items and Non-monetary items. Monetary items are those assets and liabilities the amounts of which are fixed by contract or statute in

terms of the number of rupees irrespective of the changes in the purchasing power of rupee. Items which comes under monetary in nature are as follows:

- *Monetary assets* include Investments, which are fixed in rupees, Current Assets other than Inventories.
- *Monetary Liabilities* include Secured Loans, Unsecured Loans, Current Liabilities and Provisions Since the value of monetary items is fixed in rupees, they are already expressed in terms of current purchasing power of rupee and, therefore, need no restatement.

For Calculating purchasing power gain/loss, the balance of net monetary liabilities/assets as on the date of the Balance Sheet is bifurcated into opening balance and additions/decrements thereto during the year. The opening balance is restated with reference to the index prevalent on that date. Additions/decrements are restated with reference to the average index of the year. The closing balance is deducted from the total of restated opening balance and additions/decrements. The resultant figure, if positive, is gain otherwise loss in the case of net monetary liabilities and vice versa in the case of net monetary assets.

After converting the Historical Based financial statements into Current Purchasing Power, the major financial ratio has been calculated. The calculated ratios are presented in Table-2.

DATA ANALYSIS AND DISCUSSION

IMPACT OF INFLATION ON LIQUIDITY RATIOS

These ratios are calculated to comment upon the short-term paying capacity of a firm or a concern's ability to meet its current obligation. The important liquidity ratios are current ratio and quick ratio.

Statistical Outcome of Liquidity Ratios

Table-3 summarizes the results of Liquidity Ratios under HCB method as well as CPP method from 2004-05 to 2008-09 by the help of descriptive statistics and t-test.

Descriptive statistics and t-test for the current ratio provide that mean of reported current ratio is less as compared to that of the inflated; leading to the conclusion that liquidity position of sample companies is better under CPP method. On the contrary, lower standard deviation for reported current ratio as compared to inflated current ratio clearly indicates that former is more consistent than the latter. Even though value of kurtosis is found to be more than 3 under both the methods, it is higher in CPP as compared to HCB method. Therefore it can be concluded that the inflated current ratio is more peaked than that of the reported current ratio. Yet again, the correlation value is 0.9998 represents high degree of positive correlation between both the methods. The p-value of 0.0188, which is less than 0.05, indicates a significant difference in the value of current ratio between HCB and CPP methods at 5 percent level of significance.

Hence in the case of Current Ratio our hypothesis (H_{03}) is rejected as there is a significant difference between two accounting methods.. The Descriptive statistics and t-test analysis for the quick ratio in Table-3 reveals that the mean, standard deviation, kurtosis, skewness and all other findings are the same under both the accounting methods (HCB and CPP). It is because inventory is taken away from current assets for finding out the quick assets, the result indicates the reported and inflated quick ratios are identical.

IMPACT OF INFLATION ON PROFITABILITY RATIOS

This group of ratios measures the overall performance and effectiveness of the firm. The main profitability ratios include Gross Profit Margin, Operating Profit Margin, Net Profit Margin, Return on Investment and Dividend Payout Ratio etc.

Statistical Outcome of Profitability Ratios

Generally, profitability ratios measure the financial efficiency of firms in different ways. The descriptive statistics as well as results of t-test of profitability ratios viz. gross profit margin, operating profit margin, net profit margin and return on investment both under HCB and CPP methods from 2004-05 to 2008-09 is given below in Table -4.

The Table-4 clearly shows that mean value of gross profit margin is higher in the reported (HCB) method as compared to inflated (CPP) method for sample companies over the period of study (from 2004-05 to 2008-09), meaning thereby reported gross profit margin has performed better than inflated gross profit margin. But the HCB gross profit margin has more variation than that of the CPP, since both standard deviation as well as variance shows higher value in HCB method than CPP method. Though, the distribution of gross profit margin are found to be positively skewed in both the methods, the CPP gross profit margin is little bit higher skewed than that of the HCB gross profit margin. These ratios are observed to be platykurtic by nature i.e. it is more flat on HCB method. The p-value of 0.0024 in case of gross profit margin indicates significant difference in the absolute value of gross profit margin between reported and inflated at 5% degree of significance.

In case of operating profit margin, the mean value under CPP method is less than the HCB method, disclosing thereby operating profit margin has reported at a higher value in comparison to actual operating profit margin adjusted to inflation. The standard deviation of reported operating profit margin is less than inflated which reveals that there is less variation in reported operating profit margin in comparison to inflated. Skewness of operating profit margin found to be positive in case of HCB method, where as it is negative in case of CPP method. So HCB operating profit margin is positively skewed and for CPP it is negatively skewed. The p-value shows a significant difference between reported and inflated with respect to operating profit margin. The factors influencing the inflation were tested for the degree of relationship among them to find whether the fluctuation in one factor affects the other factors. To identify the same, the factors were measured for bi-variate correlation with respect to each other and their coefficients were given in the Table-4. From the Table-4, it is clear that there is a significant correlation existing between the factors of operating profit margin of reported and inflated.

Similarly, the mean of net profit margin is higher in case of HCB method as compared to CPP method. The variation of reported net profit margin is less than the inflated net profit margin as both standard deviation and variance is found to be less in HCB method. Here too there is a significant difference between reported and inflated net profit margin as the p-value is less than 0.05. However the skewness under both HCB and CPP method was found to be negative. So it can be said that net profit margins are negatively skewed. Net profit margins under both the methods experimented to be leptokurtic by nature i.e. they are peaked.

From the Table-4, it is evidenced that Return on Investment (ROI) has executed the same trend like that of gross profit margin, operating profit margin and net profit margin. The mean value and the standard deviation of Return on Investment (ROI) under HCB method is found higher than that of CPP method. Therefore there is less consistency in case of reported return on investment. The value of p shows that there is a significant difference between reported and inflated return on investment among the two accounting methods (HCB and CPP) for the study period. While in the case of skewness both reported and inflated return on investment are positively skewed and HCB return on investment is higher than the CPP return on investment. Both the reported and inflated returns on investment are leptokurtic by nature. The HCB return on investment is more peaked than the return on investment of CPP.

Table 4 shows the results of the profitability ratios, where it can be observed that the entire profitability ratios have dropped significantly. This shows that inflation adjustment leads to impact upon the shareholders' funds. The 3rd hypothesis does suggest no significant difference between the ratios of two groups (HCB and CPP). But the p-values of 0.0024, 0.0003, 0.0000 and 0.0006 respectively for gross profit margin, operating profit margin, net profit margin and return on investment shows that there is significant difference between reported and inflated profitability ratios. Therefore hypothesis (H_{03}): 'there is no significant difference in reported and inflated financial ratios' is rejected.

IMPACT OF INFLATION ON ACTIVITY RATIOS

Activity ratios are calculated to measure the efficiency with which the resources of a firm have been employed. These ratios are also called turnover ratios because they indicate the speed at which the assets are being turned over into sales.

Statistical Outcome of Activity Ratios

Activity ratio is a very important tool to measure the velocity of current assets of an organization and includes generally Creditor Turnover Ratio, Debtor Turnover Ratio and Inventory Turnover Ratio. The details of descriptive statistics and t-test of these ratios for sample companies under HCB method as well as CPP method are given away in Table -5 for the period under study.

It is observed from the Table -5 that the creditor turnover ratio has performed better in the case of CPP method as compared to HCB method, which indicates creditors are treated well in case of inflationary condition. The standard deviation as a measure of variation is found to be higher in CPP creditor turnover ratio than that of the HCB. Again, the creditor turnover ratio under both the methods is found to be positively skewed, but it is more skewed under CPP method than the HCB method. The ratio is experiential to be platykurtic by nature i.e. it is more flat in case of HCB method. As the p-value comes to 0.0000, so it is concluded that there is significant difference in creditor turnover ratio under both the accounting methods under discussion. Similarly, it is observed from the Table-5 that the mean value of debtor turnover ratio is superior under the CPP method as compared to that of HCB method but having more variations (as the standard deviation is found to be higher). Thus it can be said that inflation has favorable impact debtors of the sample companies during the period of study. Yet again the ratio is found to be positively skewed and leptokurtic under both the methods of accounting, but more skewed as well as more peaked under the HCB method than CPP. Like the creditor turnover ratio, there is significant difference in values of this ratio under both the accounting methods since value of p is found to zero.

On the contrary, The mean value, standard deviation as well as variance of inventory turnover ratio is found to be higher in HCB method as compared to the CPP method implying that the production efficiency of sample companies has suffered to greater extent due to inflation, but it is inconsistent during the period of study. Here also, like other turnover ratios, we found the inventory turnover ratio is positively skewed under both the methods and marginally more peaked under HCB method. There is also significant difference in values of inventory turnover ratio under both the accounting methods as evidenced from the p-value.

As the p-values for all three activity ratios (Creditor Turnover Ratio, Debtor Turnover Ratio and Inventory Turnover Ratio) are found to be equal (0.0000), there is a significant difference in between two accounting methods. For this reason hypothesis (H_{03}) for Activity Ratios is discarded.

CONCLUSION

From the above discussion and interpretation of the descriptive statistics and t-test of key financial ratios, undoubtedly it is observed that inflation has affected all the ratios under study except the quick ratio. With the

pressure of inflation the current ratio, creditor turnover ratio and debtor turnover ratio have changed and performed better, but no change has occurred to the quick ratio. Nevertheless all the profitability ratios and inventory turnover ratio have suffered badly due to the impact of inflation. The financial ratio analysis thus confirms that historical accounts overstate profitability and understate liquidity.From the above discussion, it is clear that due to inflation the profitability of sample companies has been understated, resulting additional payment of tax and dividend, but reduction in shareholders' funds by dropping retained earnings. Moreover, the dismal performance revealed under the CPP method points towards the efficiency of the management in fighting against inflation. Whatever view one takes, no one can deny that, but inflation has taken its toll. The reason for overstatement of corporate profitability under HCB method may be attributed to undervaluation of material cost and depreciation. The performance which otherwise appears to be quite good, turned out to be very dismal, when adjustments for current purchasing power of rupee are made. The CPP method adjustments have thus proved that historical profitability is a fairy story.

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Table No. – 1 Wholesale Price Index in India [2000-09]

Year	Average	Average as per 2004-05	Year End	Year End as per 2004-05
2000-01	83.19	100.00	84.00	100.00
2001-02	86.18	103.59	85.48	101.76
2002-03	89.12	107.13	90.60	107.86
2003-04	93.98	112.97	94.93	113.01
2004-05	100.07	120.29	100.00	119.05
2005-06	104.50	125.62	105.70	125.83
2006-07	111.40	133.91	112.80	134.29
2007-08	116.60	140.16	121.50	144.64
2008-09	126.00	151.46	123.50	147.02

Table No. – 2 Ratios Used in the Study

Liquidly Ratios	Profitability Ratio
Current Ratio	Gross Profit Margin
Quick Ratio	Operating Profit Margin
Activity Turnover Ratio	Net Profit Margin
Debtor Turnover Ratio	Return on Investment
Creditor Turnover Ratio	Dividend Payout Ratio
Inventory Turnover Ratio	

Table No. – 3 Statistical Results of Liquidity Ratios

Particulars	Current Ratio		Quick Ratio	
	HCB Method	CPP Method	HCB Method	CPP Method
Mean	2.1681	2.2620	1.2038	1.2038
Standard Deviation	3.0700	3.3454	0.7239	0.7239
Sample Variance	9.4249	11.1917	0.5241	0.5241

Kurtosis	34.5451	35.3145	1.2978	1.2978
Skewness	5.6496	5.7361	1.2626	1.2626
Pearson Correlation	0.9998		1.0000	
Hypothesized Mean Difference	0.0000		0.0000	
t Stat	-2.1502			
P(T<=t) one-tail	0.0188			
t Critical one-tail	1.6839			
P(T<=t) two-tail	0.0376			
t Critical two-tail	2.0211			

Table No.-4 Statistical Results of Profitability Ratio

Particulars	Gross Profit Margin		Operating Profit Margin		Net Profit Margin		Return on Investment	
	HCB	CPP	HCB	CPP	HCB	CPP	HCB	CPP
Mean	0.3348	0.3232	0.1069	-0.0617	0.0618	0.0032	0.4169	0.1551
St. Deviation	0.2616	0.2606	0.1231	0.3359	0.1030	0.1581	1.3087	0.3215
Sample Variance	0.0684	0.0679	0.0152	0.1128	0.0106	0.0250	1.7127	0.1034
Kurtosis	-0.8664	-0.8272	2.4558	2.4587	8.4900	18.0787	40.1024	14.1382
Skewness	0.4850	0.5277	0.0393	-1.7679	-1.8331	-3.5369	6.2678	3.1014
Pearson Correlation	0.9953		0.5010		0.9212		0.5676	
Hypothesized Mean Difference	0.0000		0.0000		0.0000		0.0000	
T Stat	2.9901		3.7177		5.1103		3.4662	
P(T<=t) one-tail	0.0024		0.0003		0.0000		0.0006	
T Critical one-tail	1.6839		1.6839		1.6839		1.6839	
P(T<=t) two-tail	0.0048		0.0006		0.0000		0.0013	
T Critical two-tail	2.0211		2.0211		2.0211		2.0211	

Table No. -5 Statistical Results of Activity Ratios

Particulars	Creditor Turnover Ratio		Debtor Turnover Ratio		Inventory Turnover Ratio	
	HCB Method	CPP Method	HCB Method	CPP Method	HCB Method	CPP Method
Mean	3.7426	4.0907	22.9793	25.1120	11.4766	11.1810
Standard Deviation	2.8469	3.1267	23.7664	25.9161	7.8027	7.5617
Sample Variance	8.1050	9.7761	564.8427	671.6457	60.8817	57.1790
Kurtosis	-0.1930	-0.0783	5.3379	5.2297	3.1295	3.0977
Skewness	0.7862	0.8134	2.2205	2.2088	1.5887	1.5714
Pearson Correlation	0.9997		0.9998		0.9994	
Hypothesized Mean Difference	0.0000		0.0000		0.0000	
t Stat	-7.5652		-6.0256		5.5831	

P(T<=t) one-tail	0.0000		0.0000		0.0000	
t Critical one-tail	1.6839		1.6839		1.6839	
P(T<=t) two-tail	0.0000		0.0000		0.0000	
t Critical two-tail	2.0211		2.0211		2.0211	

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RESEARCH ARTICLE

Green Synthesis of Metal Nanoparticles and its Characterizations: A Review

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ABSTRACT

The primary focus of this review is to highlight the recent advances made in the field of nanotechnology. Essentially, it includes the green synthesis of metal nanoparticles (NPs), which has significant socio-economic benefits. Being an economically viable and bio friendly approach, green synthesis of nanoparticles is the need of the hour. Since time immemorial, plants are gifted with several phytochemicals like polyphenols, terpenes, sterols, carotenoids, vitamins and many more which have innumerable beneficial effects, one of which is their reducing attribute, resulting in the reduction of metal salts to their corresponding metal Nanoparticles (MNPs). Plant parts including bark, leaves, fruit, seed, root, flowers exhibit diverse medicinal potentials including anticancer, anti-inflammatory, antidiabetic, antioxidant, antibacterial and antifungal properties. The phytochemicals present are responsible for both preparation and stabilization of metal nano particles. These phytochemicals also act as capping agents to restrict the metal nano-particles for agglomeration which may produce less reactive big size metal nano particles. The prepared MNPs were examined by UV-Vis, FTIR, XRD,DLS,SEM, TEM, EDAX and Zeta potential analysis. In this preview, a comprehensive study on the preparation, characterization and antimicrobial activity has been portrayed. A detailed perspective of anti-microbial activity against several pathogens is also outlined. This study can be a stepping stone for developing novel NPs.

Keywords: Nanoparticles,Green synthesis, anti-inflammatory, Anti-microbial study

INTRODUCTION

From last few decades different valuable applications in different field of science have been found in nanoscience and different branches of scientific research are undertaken in this field of science. The word "Nano" came from the Latin word nanus means dwarf with particle size of 10^{-9}meters. The size of nanomaterial are between molecular &

macroscopic dimensions. i.e. greater than 1nm and less than 100nm.Different interdisciplinary applications were discovered by advance scientific research on nano-sciencelikeapplication in the field of data storage, biomedicine, catalysis, energy technology, magnetic and fuel cells. Due to the vast application of nanotechnology it received growing interest in this century. Nanoparticles (NPs) are minute particles with dimension lies below 100 nm (1 nm = 10^{-9} m). They possess excellent physical, chemical and biological properties which make them special in the field of materials science and biology. The synthesis, study and applications of various NPs are highly essential in science & engineering. Based on the size, morphology, physical and chemical properties these have different application mainly in the field of medicine or therapy. The conventional synthesis of MNPs have various risks to the environmentby consuming chemicals and by liberating hazardous chemicals or gases to the environment. The physical route involves high energy consumption and the chemical route generally involves use of toxic chemicals & release of hazardous byproducts.So green synthesis or bio-synthesis isan excellent alternative route for the synthesis of nano-samples by overcoming the drawbacks of physical & chemical methods. The recent introduction of biological methods involves microorganisms, algae, or plants at ambient temperature and pressure in a bio-friendly manner. Out of these green synthesis routes, the use of plants and its different parts have proved most convenient and economic. The phyto-chemicals containing different bio-molecules present in extracts of different parts of plant are responsible for the reduction of positively charged metal ions into atomic or nano form (in nano size) which are helpful in stabilizing the synthesized aggregateatoms before the production of nano scale particles.

Because of unique properties of NPs like large surface area,adsorption, quantum and releasing properties, the NPshave showed a great potential in interdisciplinary applications. NPs are broadly classified as carbon-based NPs (Graphene, fullerenes carbon nanotubes etc.), ceramic NPs (SiC, BN, Al_2O_3, etc.), metal NPs (e.g., gold, silver, platinum, copper, etc.), oxide NPs (e.g., Cuprous oxide Cu_2O, Zinc Oxide ZnO, Titanium oxide TiO_2, etc.), semiconductor NPs (e.g., GaP, GaAs, GaN etc.) etc. The size, morphology, dispersibility and physicochemical properties of MNPs are depends on its synthesized routes which in-turn depends on its different interdisciplinary applications.Thus, the main objective of recent MNPs research is to find host which may control the properties of MNPs.

According to Hett, (2004) Nanoparticles are classified into three categories. Such as One, two& three dimension. One dimension or primary NPs are surfaces or thin film which is used in engineering electronics and chemistry. Thin films are recently used in Solar panels or solar cells or used as catalyst. Secondary or two dimensionalNPsmainly includes Carbon nano-tubes (CNTs). These have hexagonal structure with diameter of 1 nm and length of 100 nm.These are of two types. (a) single-walled carbon nano-tubes (SWCNTs) and (b) multi-walled carbon nanotubes (MWCNTs). Kohler et al., 2004 reported the unique properties of CNTs like physical, mechanical and electrical properties which make them chemically very stable.The best example of tertiary or three dimensionalNPsis Fullerenes (C_{60}).These have 28 to more than 100 carbon atoms connected through a pentagon or a hexagon resembles a spherical cage or a soccer. These have unique physical & chemical properties.It is used in solar cells for data storage.Tomalia, 2004 have reported the presence of large empty spaces for guest bio-active molecules which may show significant medical applications.

Preparation of Metal Nano Particles (MNPs)

The physical, chemical and biological properties of nanoparticles with size,structure depends on its synthesis method.The various factors which affect the particle size, chemical composition, crystallinity and shape are pH, concentration of precursor salt solution, temperature, concentration of capping agent, sonication conditions, etc. Various shapes of MNPs are reported & characterized like nano cubes, nano triangles, nano tetrapods, nano stars, nano cluster, nano branch, nano rod, nano sphere, nano wire, nano tripod, nano prism, nano disks, nano shells, nano frames. Therefore, the selection of preparatory route & condition are important in preparation of desired nanoparticles.

The two basic routes employed to prepare NPs are: (1) Top-down methodand (2) Bottom-up method1. In the top-down method, NPs are obtained by mechanical crushing of source material. Some examples are high energy ball milling, laser ablation, electro-explosion, chemical etching, etc. In the bottom-up method, by chemical or physical process new structures are built up . Here NPs are obtained as aaddition of atom to atom or molecule to molecule addition. This route is based on physio-chemical principles which follow atomic or molecular self-organization. Some of the examples of this route are sol-gel process, green synthesis, chemical reduction method, hydrothermal route, chemical vapours deposition (CVD), combustion, aerosol process, plasma spraying process, etc.

Green synthesis of noble metal NPs & its Characterization- review

The use of chemical & physical methods for the synthesis of MNPs leads to high energy consumption or use of toxic chemicals or generation of hazardous by-products. In chemical method, the toxic capping agents present do not show any biomedical applications. Alternatively, use of bio-synthesis routein spontaneous condition and nontoxic environment can maintain ecological integrity & eliminate the drawbacks of conventional approaches.

The various common conventional routes mentioned earlier in synthesis of NPs utilize toxic chemicals which are not environmental benign. So, now-a-days researches in the field of biology, chemistry, and materials science are adopting bio-directed synthesis (also known as green synthesis) of NPs. Biosynthesis of MNPs is an eco-friendly route which avoid utilization of hazardous, carcinogenic, harsh chemicals. The various biological methods employ micro-organisms (algae, bacteria, fungi, yeast, etc.) and various plant parts in synthesis of NPs. As plant mediated synthesis is cost effective, it is widely used in these days for macro scale synthesis of MNPs. Also the various phyto-chemicals present in plant extracts are acts as both reducing and stabilizing agent in developing MNPs.

Abbasi et al.[1] have synthesized spherical Gold nanoparticles (GNPs) of well defined morphology from aqueous extract of *guduchi (Tinosporacordifolia)*. Depending upon the ratio of extract concentration and metal solution, two types of the surface plasmon resonance (SPR) band was found to be under UV-Spectra. first peak as a single peak in the visible region with λ_{max} 551 nm , and the second peak as a double was found as two peaks with λ_{max} at ca. 555 and 980 nm.Due to presence of aliphatic nitro group , a strong absorption band was obtained under FTIR spectra. In XRD study, the structure of Gold nanoparticles (GNPs)was found to be Face Centred Cubic with crystallite size ranging from 22.3 to 51.4 nm. SEM and HR- SEM predicted the Au NPS were of spherical shape having size ranges from 16–30 nm& 25–75 nm both thecombination.From EDX spectra it was revealed a strong band showing thepresence of Gold nanoparticles (GNPs).Huang et al.[2] have used an aqueous chitosan extract (100% deacetylated, Fluka). for the preparation of MNPs (Gold and Silver). Here Polysaccharides acts as reducing & stabilizing agents. The SPR band was found to be 522nmindicates the presence of Gold nanoparticles (GNPs). TEM image confirms isotropic nature of synthesized particles.

UjjwalaGaware et al.[3] have synthesized GNPsby using an aqueous solution of Piper betleleaves. By UV-Visible characterization it is seen that the Surface Plasmon bandλ_{max} at 551nm which intensity increases steadily which indicates the presence of spherical GNPs .There was found a reduced absorption band in FTIR spectra which revealed the interaction of phyto-chemical present as aldehydes orketones with the Gold nanoparticle . From XRD analysis indicates the Au NPs having fcc structure & crystalline in nature.The triangular shape of GNPs was confirmed by TEM with edge-length660nm to 1000nm. "Lightning-rod effect" indicates the presence of MNPs with anisotropic properties. Yong Song et al.[4] have reported the synthesis of GNPs from Diopyros kaki and Magnolia Kobus with variation in temperature. There is no significant change in FTIR spectra was observed before and after the bio-reduction inMagnolia Kobus leaf extract. Thepresence of multiple functional groups in Kobus is responsible for the synthesis of GNPs. TEM images shows a mixture of plate (triangles, pentagons, and hexagons). With increase in concentration of leaf extract, the particle size of GNPs increases. With rise in temperature, the particle size decreases i.e. at 25 ^{0}C the particle size was found to be 110nm but at 95 ^{0}C it was found to be 40nm. From Atomic Force Microscope (AFM) study it was revealed that, the synthesized GNPs showing structure like nanoplates having

width of 250–300 nm and thickness of 5-7nm in 5% Magnolia leaf broth at 25^{0}C. EDX spectra it was revealed a strong band showing the presence of GNPs. XPS spectrum revealedsynthesis of GNPs by bio-synthesis using plant leave extract.

Shiying He et al.[5] have utilized Microorganisms and Culture Conditions for the synthesis of Gold nanoparticles (GNPs).Amixed culture of Rhodopseudomonascapsulatain a medium withyeast, pyruvate, extract, NaCl, NH_4Cl, and K_2HPO_4 at pH 7 and 30 °C are used for the synthesis purpose of Gold nanoparticles (GNPs) .The SPR band with a strong absorption of 530nm confirmed from UV-Visible spectra. The GNPs are found to be isotropic and uniform size.From the FTIR spectrum, band at 1640 and 1540 cm^{-1} indicates the presence of amide and band at 1450 cm^{-1} showing the presence of methylene scissoring vibrations in proteins. The synthesized GNPs were stabilized by binding of amine or cysteine residue part of protein. From TEM image the size of synthesized GNPs ranging 10-20 nm qt lower concentration of auric acid solution i.e. concentration of 2.5 $x10^{-4}$ M and from selected area electron diffraction (SAED) pattern by TEM pattern the synthesized GNPs were shown. From XRD analysis a characteristicpattern of face-centred cubic (fcc) was obtained for synthesized GNPs by using Scherrer equation. From EDAX spectrum, astrong signals confirms the presence of Gold nanoparticles (GNPs). Das et al.[6] have utilized alcoholic (ethanol extract) of Centellaasiatica leaves for the synthesis of GNPs of well-defined size and distinct morphology. Thephyto-chemical present in the extract with high phenolic content with anti-oxidant nature help in reduction of Gold salt GNPs. The synthesised NPs were characterized using UV–visible spectra with SPR band at 534nm, Ultra High Resolution Transmission Electron Microscopy (UHR-TEM) shows formation of spherical NP, Fourier Transform Infrared (FTIR) spectrophotometer shows the distinguished interaction between Gold salt and phyto-chemical present in plant extract. X-ray diffraction (XRD)revealed the synthesized Gold nanoparticles (GNPs) have face centred cubic (FCC) array of crystal.

Isaac et al.[7] have used fruit extract of Averrhoabilimbi Linn for the synthesis of GNPs and Silver nanoparticles (SNPs).UV-Visible spectra showed SPR band at 540nm for GNPs and 420nm for SNPs. FTIR spectra revealed characteristic strong absorption bands which confirmed the interaction between metal salt and phyto-chemical present in the extract. The C–OH stretching of primary alcohols, the silver showed bands at 3285, 1633, and 1025 cm^{-1} assigned to O–H stretching vibration of alcohols and phenols, C=O stretching vibration of Tertiary amides, and C–OH stretching of primary alcohols. Scanning Electron Microscope (SEM) confirms the presence of anisotropic MNPs (i.e., cubic, hexagonal, pentagonal, etc.). Patra et al.[8] have reported synthesis of GNPs from the water extract of watermelon grid and evaluated their antioxidant and antibacterial effects.They reported that synthesized GNPs have significant antibacterial potential against five foodborne pathogens (i.e.Bacillus cereus, Escherichia coli, Listeria monocytogenes, Staphylococcus aureus, Salmonella typhimurium.). The Au nano colloids exhibited high synergistic activity against the standard antibiotics like rifampicin & kanamycin. The synthesized GNPs have considerable anti-proteasome, antioxidant and inhibitory potential against standard antioxidant. They analyzed the effect of reducing and stabilizing character of phytochemicals present in the extract using FTIR. To confirm the formation of Gold nanoparticles (GNPs), they took the help of results obtained from Ultra Violet–Visible spectra, SEM and EDAX plot. Kumar et al.[9] have reported synthesis of GNPs using extract Zingiberofficinale. The size of the synthesized GNPs was 5-15 nm. Due to its physiological stability and active good blood biocompatibility, these may be used in medical applications. The synthesis of GNPs with size distribution wasconfirmed by using dynamic light scattering DLS, UV–Visible spectrophotometer and TEM. Islam NU et al.[10]utilized galls extract of Pistaciaintegerrima for the synthesis of GNPs. The prepared AuNPs reported to exhibit good antifungal activity and possessed superior muscle relaxant property. Kumar et al.[11] have preparedSNPs) by using finely grounded powder of Mimusopselengifruit extract in water. The synthesized samples were characterized by using different spectroscopies (UV-Visible, FTIR and TEM). The synthesized SNPs have significant antibacterial and antioxidant properties against Escherichia coli (E. coli) &Staphylococcus aureus (S. Aureus) pathogens. Also the synthesized SNPs are reported to act as good antioxidant against ascorbic acid.

Majumdar et al.[12] have reported the synthesis of colloidal GNPs by using aqueous bark extract of Mimusopselengi. The characterization of synthesized colloidal GNPs were done by using UV-Vis, TEM, and X-ray diffraction (XRD). From the UV-visible spectra, the synthesized GNPs have SPR band between 536nm to 541 nm and spherical shape. The XRD analysisconfirmed the presence of GNPs with face-cantered cubic (FCC) array pattern. They reported the phyto-chemical present as poly-phenols in the extract showed both reducing as well as stabilizing properties confirmed from FTIT studies.J. Kasthuria et al.[13]revealed green synthesis of GNPs and SNPs utilizing apiin. They reported apiin has reducing character which helps in synthesis of MNPswith varying concentration of apiin extract. From UV-Visible spectra, a well separated two SPR bands were obtained at 540nm (spherical) and 950nm (plannar). For SNPs SPR band is at the 456nm. The FTIR analysis shows bio-reduction of metal salts ($AgNO_3$ and $HAuCl_4$) with phyto-chemical present in the extract. The lower frequency shift in GNP) revealed the effective adsorption of apiin extract on GNPs than SNPs. TEM image reported maximum presence of spherical particles than triangular ones. The presence of different sized nanoparticles were 7.5nm range (30%) and 12.5nm range (54%) range and 23 nm ranges(12 %) and 65nm (small %). XRD analysis of the synthesized Gold nanoparticles(GNPs)from apiin extract was found to have Face Centred Cubic(FCC) pattern. The single crystallinity of the synthesized particles was confirmed from selected-area electron diffraction (SAED). The average size of the synthesized GNPs was 39 nm with quasi-spherical shape.The presence of water molecules in the synthesized MNPs was confirmed by TGA analysis with a steady loss of weight until 800°C.

Fakayode et al.[14] have reported the synthesis of Noble Metal Nanostructures by using non-polysaccharide reductants like Sodium citrate, Sodium Borohydride ($NaBH_4$), Tetrakis (Hydroxymethyl) Phosphonium Chloride (THPC) &polysaccharide reductants like Starch, Cellulose, Dextran. The absorption peak of SPR band from UV-spectra was 520nm for GNPs and 400nm for Silver nanoparticles (SNPs). From FTIR data analysis, the interaction between polysaccharide and GNPs or SNPs was confirmed by wave-number absorption bands. From zeta potential data it was confirmed that the synthesized gold and silver NPs were surrounded by negative charges. The positively charged polysaccharide based gold and silver nanoparticles were stabilized by electrostatic repulsion of the polysaccharide's molecules. Dynamic Light Scattering data revealed that size of the synthesized gold and silver nanoparticles decreases with concentration rise of polysaccharide to a certain extentand due to aggregation it increases further at high concentration. The synthesized NPs are characterized using TEM, SEM and XRD. The synthesized sample containingGNPs are used in medical applicationlike plasmonic bio-sensing detection, bio-imaging, fluorescence detection, Photo-thermal Therapy and the synthesized sample containing SNPs are used in medical application like Diagnostic enhancement, Targeted antimicrobial activity, Anti-angiogenesis activity.

Dubeya et al.[15]synthesized colloids of gold and silver by utilizing aqueous leaf extract of Sorbusaucuparia. From UV–vis spectra, the SPR band was found to be 300-1000nm for GNPs and 400-1000nm for 400nm for SNPs which is confirmed by the colour change from brown–yellow for silver and pink–red for gold. TEM images analysis revealed that the particle size was 50-100nm for Silver and 50-150nm for GNPs of nanoparticles at 10^{-2}, 10^{-3} and 10^{-4}M concentration of SNPs. Zeta potential value rises with increase in pH of the solution for Silver but samples with gold solutionhad no effect of change in p^H on zeta potential value. Both synthesized nanoparticles have negative zeta potential value over a wide range of p^H. FromPowder XRDdata it was revealed that both Gold and Silver samples have FCC crystal array. The presence of Gold and silver was confirmed by EDX study. FTIR absorption band indicates theinteraction and stabilization of bio-synthesized MNPs.

Faramarzia et al.[16]synthesizedGNPs utilizingaqueous extract of laccase from Paraconiothyriumvariabile. Laccase of P. variabile is purified, assayed & the temperature stability is determined by incubating at different temperatures. By increasing the concentration of Chloroauricacid, increases the absorbance to 520 nm.The best result of size range between 71-266nm was found at 70 ^{0}C after incubation time of 20minutes. From FTIR analysis, two major absorption peaks were obtained which corresponded to alcohol or amine or carbonyl functional groups present as phyto-chemical. The data from SEM, TEM and EDX confirmed the presence of GNPs.Shih et al.[17]reported the synthesis of GNPs using alkaline solution of chitosan. The synthesized samples were studied under different spectroscopic

techniques. They reported the decrease in synthesized particle size with respect to concentration change of polysaccharide. Sunet al.[18] synthesizedGNPs using biopolymer in acidic medium in presence of chitosan. The mechanism of formation of nanoparticles is reduction to open chain. The applicability of chitosan in preparation of GNPs was studied and by peptide synthesis and protein many preparatory ways have been developed.

Khalil et al.[19]have demonstrated bio-synthesis of GNPs fromaquousleaf extract ofOlive. From UV-Spectra, SPR absorption band was545 to 530 nm. Photoluminescence studies revealed emission at 425nm at an excitation of 350nm. The TEM image revealed that formation of triangular shaped GNPs with diameter of 50 -100 nm. The FTIR study showed the probability of binding of synthesizedGNPs with antioxidant group or protein present in extract as phyto-chemical. X-ray diffraction study revealed the presence of crystalline GNPs were identical with blue shift spectra at basic pH of 9.6. pseudo-spherical shaped GNPs were seen at higher extract concentration and p^H. The synthesized GNPs were well interacted and stabilized or capped by phyto-chemicals present in extract. The synthesized samples have many bio-medical applications because no toxic reagents had been used in synthesis. Daizy Philip[20] has reported biosynthesis of GNPs & SNPs using aqueous extract of Mushroom. UV absorbance spectra showed SPR band at 545nm for the gold colloids with size of the NPs range from 20 to 150 nm. With excess of the NPs there is formation of spherical shaped NPs by agglomeration. FTIR studies revealed that the interaction between bio-molecules as phyto-chemical present in extract and metal salt which may acts as both stabilizing and capping agent. Due to this the surface of the GNPs prevents the sintering of nascent gold nano-crystals. The SPR band from UV–vis spectra of silver colloids was found at 413 nm. The XRD study confirmed the crystalline structure of gold nanoparticles. Photoluminescencespectra showed emission at 300nm of the synthesized GNPs at an excitation of 300 nm.

The study reported by B.Ankamwar[21] is synthesis of GNPs using aqueous extract of Terminalia catappaleaves. The SPR absorbance band from UV-spectra was found to be at 524nm. FTIR spectra indicate the possible interaction between bio-molecules in the leaf extractand the Gold salt & the stabilization of synthesized GNPs was due to phyto-chemical and capping agents present in the extract. TEM image showed synthesized GNPs were spherical in shape with size of 10 - 35 nm at an average size of 21.9 nm.XRD analysis showed the synthesized Au NPs have FCC structure & the antimicrobial, antioxidant properties have application in cancer therapy. Inbakandana et al.[22] reported synthesis of GNPs utilizing marine sponge Acanthella elongate. The SPR band was appeared at 526nm. TEM image indicates the synthesized GNPs were seen as poly-dispersed with spherical shape with size range of 7 to 20 nm. FTIR data showed strong absorption band by the interaction of phyto-chemical with metal salt solution.

Sastry et al.[23] have reported biosynthesis of metal nanoparticles (both Gold and Silver)using fungi and actinomycete. The synthesized SNPs were prepared by intracellular synthesis by using Verticilliumsp.(from the Taxusplant)base of potato-dextrose agar slants at 25°C. TEM images of reported the particle diameter of 25 ± 12 nm.GNPs undergo extracellular synthesis byactinomycete, Thermomonospora sp. with a much improved polydispersity.UV-Visible spectra revealed SPR band at 520 nm. FTIR spectrum recorded two strong absorption bands 1660 and 1530 cm^{-1}. TEM images showed that the synthesized GNPs have spherical shape with average size of 8nm. The Synthesized GNPs are mono-dispersing in nature. Huang et al.[24]synthesized GNPs and SNPs by using leaf extract of Cinnamomumcamphora. The leaf extract were sun dried and novel in nature and commercially available noble metal salts ($AgNO_3$ and $HAuCl_4$) were used for the synthesis of MNPs. From UV-Visible studies the SPR band was at 570 nm & 440nm for Au & Ag NPs respectively. The poly-dispersity of the synthesized MNPs was confirmed by TEM image. TEM image also revealed the anisotropic nanostructures of synthesized MNPs. The crystalline nature of synthesized MNPs was confirmed by XRD studies. A.Thirumurugan et al.[25] have reported biotechnological preparation of GNPs utilizing aqueous extract of Azadirachta indica leaves. The SPR band was at 550nm by using UV-Visible spectra.

Badri Narayanan et al.[26] have reported synthesis of GNPs by using aqueous extract of Coriander leaf. The SPR band was at 541nm by using UV-Visible spectra. XRD analysis reflects FCC structure of gold nanoparticles & by using

Bragg's equation the size was found to be 15nm. A strong peak of Gold atoms from EDAX studies confirms the presence ofGNPs and a weak signal of carbon atoms may arise from X-ray emission of proteins or enzymes present in vicinity of the GNPs. FTIR spectra showed a strong absorption bands corresponds to C–N stretching vibrations of amine. HRTEM studies revealed that the synthesized GNP have spherical, decahedral, triangle and truncated triangles shape with size ranging from 6.75 nm to 57.91 nmwith an average size of 20.65±7.09 nm. Philip et al.[27] have presented extracellular biosynthesis of GNPs and SNPs using aqueous extract of Krishna Tulsi (Ocimum sanctum) and Auric Chloride& Silver nitratehe SPR band for GNPs and SNPs were at 545nm and 426nm. TEM images showed the synthesized GNPs have hexagonal shape with average size of 30nm and the synthesized SNPs were spherical shape with particles size of 13nm. XRD analysis showed both GNPs& SNPs were having FCC lattice array. The crystalline nature of GNPs was confirmed by Selected area electron diffraction (SAED) pattern. Strong absorption bands in FTIR spectra revealed the presence of biomolecules as phytochemicals are responsible for the stabilization and capping of synthesized MNPs.

Kumara et al.[28] have reported facile bio-synthesis of GNPs using aqueous leaf extract of Cassia auriculata. The leave of Cassia auriculata has antidiabetic potential. The SPR band was at 536nm by using UV-Visible spectra. From FTIR spectra the strong interaction between GNPs and bio-molecules present in the extract was established. TEM image showed the shape of GNPs were spherical, hexagonal and triangular in shape with size range of 15–25 nm in size. XRD analysis reflects FCClattice array of synthesized GNPs. SEM image revealed the synthesized GNPs were aggregated with size range of 15–25 nm .Chen Wu et al.[29] have presentedgreen-synthesis of GNPsusing aqueous solution of Gum Arabic. The extract is both acts as reducing and a stabilizing agent. UV-Visible spectra revealed a characteristicSPRband at 534.5-532.5nm. The TEM image reflects the non-agglomeration of GNPs may be due to presence of phyto-chemical in Gum Arabic extract with a size range of 21.1±4.6nm. From DLS studies the mean hydrodynamic diameter was found to be 26.8±5.3 nm. XRD analysis showed the synthesized GNPshave FCC array of lattice .With the variation Temperature and concentration of both Gold solution & the type of GNPs synthesis were different.

Daizy Philip[30] has reported synthesis of GNPs and SNPs by using aqueous extract of Hibiscus rosasinensis and Auric chloride & Silver nitrate at different concentration with p^H change. The shape of the Silver nanoparticles changes with change in p^H of the medium. The SPR band for GNPs was 576nm& for SNPs it was 413nm. TheTEM studies revealed the synthesized GNPs were spherical in shape and anisotropic. Theparticlesarealmostsphericalwithsize of14 nm.XRD analysis confirmed the GNPs have FCC lattice array with particle size of 13nm. Similarly,SNPs also have FCC lattice array. FTIR spectral studies showed the GNPs were stabilized by amine group present in extract as phytochemical and SNPs werestabilized by carboxylate ion present as phytochemical. Dubeya et al.[31] have prepared biotechnologically Gold and Silver nanoparticles utilizing aqueous leaf extract of Rosa rugosa. The UV-Visible spectra revealed that the SPR absorption band for GNPs was 578nm and for SNPs was 451nm with colour change frompink-red colour and brown-yellow respectively. TEM images study confirmed both the synthesized MNPs were spherical in shape with particle size of 30–60 and 50–250nm in case of SNPs and GNPs. Zeta Potential data showed that the synthesized MNps were stable in a pH range of 2-10 and the negative zeta potential value increases with increase in pH.The average crystal size of SNPs and GNPs were 12nm and 11nm revealed from Powder X-ray diffraction studies by Scherrer equation. FTIR spectra revealed the interaction and stabilization of synthesized MNPs with phyto-chemical present in extract.

Honey mediated green synthesis of GNPsby Daizy Philip[32] in his another paper reported the synthesis of GNPs using diluted solution of honey. The fructose and monosaccharidepresent in honey acts as reducing agent for the reduction of metal salt to metal atoms or nanoparticles. From UV-Visible spectra the SPR band of Au NPs was 576nm with characteristic of spherical particles. TEM studies showed that the synthesized GNPs are spherical in shape with average size of 15nm. Selected area electron diffraction (SAED) pattern revealed the synthesized GNPs have crystalline nature. XRD analysis revealed the FCC array of lattice with average size of 15nm by using Scherrer equation. There was no sintering of nascent Gold atoms because of strong interaction between biomolecule as

phytochemical in extract and GNPs.FTIR spectra revealed the presence of phyto-chemicals in extract have strong interaction with the synthesized GNPs which acts as both stabilizing and capping agent. Photo-luminescence spectral data showed emission spectra at around 447 nm. The synthesized GNPssamples have significant therapeutic applications.

Nora Elizondo et al.[33] have reported polyol method of synthesis of MNPs (GNPs and SNPs) using ethylene glycol as solvent redactor by using poly(vinylpyrrolidone) (PVP),Auric acid ($HAuCl_4$) (III) hydrate,Silver nitrate ($AgNO_3$) and poly (N-vinyl-2-pyrrolidone) (PVP) by use of plants like Cucurbita Digitata , Aloe Barbadensis, Rosa Berberifolia and Geranium Maculatum,. The prepared ascorbic acid from the above process acts as reducing agent. The Uv-Visible spectral data revealed that the SPR absorption band at 547nm for GNPs and 417nm for SNPs. TEM image revealed that the Spherical NPs with particle size of 29-120nm for GNPs and 10-27nm for SNPs. From precursor injection method, the synthesized silver nanoparticles(SNPs) have a uniform size of 25 ± 4 nm with high monodispersed. From Near field Scanning Optical Microscope (NSOM)studies revealed that the synthesized GNPs have a particle size of 25 nm with narrow distribution. The XRD analysis data (D-value, k= 0.90) calculated from reflection of cubic phase of Gold tally with TEM image data i.e.25nm.The spherical and quasi-spherical and monodisperse SNPs were obtained from $AgNO_3$ with Aloe Barbadensis. 4nm size of GNPs were synthesized with glycolextracts of CucúrbitaDigitata. GNPs with anisotropic nature and SNPs with spherical or quasi-spherical shape were synthesized by the reaction of Auric acid with aqueous extract of Aloe Barbadensisat 60°C and silver nitrate.

Narayanan et al.[34] have followed phytosynthesis method for the synthesis of GNPs following dilutedleaf extract of Coleus amboinicus Lour. This process of synthesis is more convenient and acceptable as microbial method is more tedious and time consuming. The UV-Visible data revealed that the SPR absorption band was 536 nm. From XRD studies, the synthesized GNPs have spherical shape with an average size of 23.7±0.72 nm and with a magnification of x23k, the average size was found to be 50-80nm. A strong peak in spot-profile EDAX revealed the presence of Gold atoms with a weak signal of carbon. FTIR data showed interaction between biomolecules present in extract with metal salt by showing a strong absorption peak. The shape of the synthesized GNPs were spherical, triangle, truncated triangle, hexagonal and decahedralwith an average size of .5±11.45 nm at a magnification of ×50 k.

MubarakAli et al.[35] have attemptedeco-friendly synthesis method for the synthesis of MNPs (GNPs and SNPs) utilizingdiluted water extract of Menthapiperitaleaves. UV-Visible data showed the SPR absorption peak at 450 nm & 530 nm for SNPs and GNPs respectively. From FTIR studies it was confirmed that the presence of bio-reducing groups as phyto-chemical in the extract responsible for the reduction of metal salt ($AgNO_3$ and $HAuCl_4$) and stabilizing with capping of synthesized nanoparticles. A broad peak at 3394cm−1 wasrevealed the presence of N–H group from any peptide bond linkage. SEM image confirmed that the synthesized MNPs (GNPs and SNPs) are spherical in shape. The average size of GNPs were150 nm. The elemental metal signal of Silver and Gold was confirmed from Energy dispersive spectroscopy (EDS) studies. The Synthesized samples having SNPs have considerable antibacterial effect on pathogen E. coli thanS. Aureus. This may be due to different cell wall composition of positive gram and negative gram (E. coli) pathogens. On the other hand,the synthesized samples having GNPs have antibacterial effect on E. coli not in S. Aureus. Whereas the plant extract has no antibacterial property. Ghosh et al.[36] have utilized the aqueous extract of *DioscoreabulbiferaTuber* for the synthesis of GNPs with anisotropy properties. The SPR peak was 540nm revealed from UV-Visible spectra. Field emission scanning electron microscope-energy dispersive spectrum (FSEM-EDS) studies revealed the shape of synthesized GNPs werespherical with diameter of 11-30nm and size of 17-18nm. Different shapes with size have been predicted form the data asnanotriangle with equilateral edges with length 270 nm approx., the average size of 207nm and the average size of trapezoids was 300 nm. The EDX studies revealed that the strong signal of gold indicates the presence of atomic gold. XRD spectra revealed the synthesized GNPs have FCC lattice array with a crystallite size of ~13 nm. FTIR spectral analysis showed interaction between phytochemical present in extract and used noble metal salt solution with strong absorption bands.

Sharma et al.[37] have synthesized GNPs fromSeeds of Sesbaniadrummondii. The seed are germinated using 85% H_2SO_4 and sterilized in 0.1% $HgCl_2$. TEM image revealed the synthesized GNPs were spherical shape with 6-20nm of average size range. EDX studies showed that the GNPs were present with agglomeration and look dense. X-ray absorption spectroscopic techniques such as x-ray absorption near-edgestructure (XANES) and extended x-ray absorption fine structure (EXAFS) were used in this study to confirm the oxidation state and form of gold in the plant tissue. XANES spectra confirmed the presence of Gold (0) oxidation state in the synthesized samples. Synthesized samples with 80-85% Gold (0) content was confirmed by LC-XANES fittings. The remaining 15–20% of gold present as gold sulphide. The presence of gold neighbours in the EXAFS is another confirmation for the presence of gold (0) in the plant samples. An absorption peak of 317nm was observed by UV-Visible spectra for the sample containing biomatrix-gold nanomaterial. This type of synthesis undergoes in situ catalytic approach. The used biomatrix nanomaterial have well defined dimensions and monodispersed. This approach may have future applications as a cell-immobilized stable catalyst.

Huang et al.[38] have synthesized MNps (GNPs and SNPs) using Chitosan. It is a polysaccharide prepared from chitin by partial deacetylation. Here the phytochemical is the polysaccharide which acts as both reducing, stabilizing and capping agent. From UV-Visible spectra, a SPR absorption band was at 522nm. SNPs were synthesized by using heparin. It acts as both reducing and stabilizing agent for the synthesis of SNPs. The SPR band was observed at 401nm for SNPs.TEM image revealed the synthesized particles are isotropic. With rise in concentration of heparin, the absorption maximum increases (451 nm). The synthesis of positive or negative charged GNPs or SNPs depends on the polysaccharides which may have many applications in the field of nano-scale superstructure fabrication.

Wanget.al.[39] have reported bio-mimeticpreparation of GNPs using the peptide sequence of MS14 (MHGKTQATSGTIQS). The synthesized GNPs are characterized by UV visible spectrometer & its SPR band was 543nm. Kalishwaralal et al.[40]have presented the bio-synthesis of Gold nanocubesusing amylase. The amylase is prepared form B. Licheniformis. It is acts as the reducing agent responsible for bio-reductionnoble metal salt to GNPs. TEM image showed the synthesized GNPsare spherical in shape with average size of 18nm. The SPR band was at 562nm. XRD reveals the synthesized GNPs are having FCC lattice array with Particle size of 14nm by using Debye Scheerr equation.

CONCLUSION AND PERSPECTIVES

Necessity is the key to invention or discovery. Day by day rapid increase of our demand or needs make research interesting. From the above reviewed discussion it is clear that biosynthesis or green synthesis has profound advantages over physical and chemical synthesis because of its eco-friendly, economic and convenient method of synthesis. The most important thing is in green synthesis no toxic chemical is used or no hazardous by-product is produced. The phyto-chemical present in different parts of plant like bark, leaves, fruit, seed, root or flowers etc. Are mostly responsible for the reduction of noble metal salt ($AgNO_3$ or $HAuCl_4$)and responsible for its stability and capping to prevent agglomeration. Due to its small size, large surface area and non-toxic nature of synthesized MNPs, these have a vast area of application in present aspect and have a bright futuristic scientific research scope. Mainly these are used in bio-medical,bio-sensing, catalysis and effective anti bacterial applications in medicine. The synthesized MNPs should be **properly** characterized using UV-Visible spectroscopy, FTIR spectroscopy, XRD, DLS, and HR-SEM and the antibacterial, antifungal, antiviral, anticanceretc.which may be used in newera of medicinal aspect.

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RESEARCH ARTICLE

Youtube, Education and the Youth: A Perceptual Analysis

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ABSTRACT

Education is considered as the backbone of a democratic society. For the better future of a democratic society, education is highly essential. The process of educating never ends with teaching rather it is completed with learning. The process of learning is completed by internalization of the subjects and their application in everyday life. The new generation students are quite different by their attitude and they are highly techno savvy. Learning through the class room teaching has become a task of boredom for them and at the same time they want education to be imparted in an attractive and interactive form.

In a country like India where education for all has still remained a challenge, providing education through attractive means is also a bigger question and a necessity of the hour. To provide education in a powerful manner there is a need of providing it to people through a user friendly and attractive medium to make learning interesting. These days along with entertainment, the biggest video platform YouTube has become popular among youth as the most popular communication platform which can play a major role in this regard and the study here is an attempt to provide an understanding about the perception of youth relating to YouTube as a learning platform.

Key Words: Social Media, knowledge, information, Development, Technology

INTRODUCTION

Wilber Schramm in his famous book *"Mass Media and national development"* (1964) says "Light is better than darkness and knowledge is better than ignorance". So knowledge is an essential requirement for human beings to survive in a society and education is the means for knowledge. Socrates speaks "Education is the kindling of a flame, not the filling of a vessel", It means education should be provided in such a way that it should inspire the students to gain more and more knowledge. It should help them to empower themselves by learning skills of life. It should help them to solve the challenges of life with the knowledge they have received from their education.

While discussing the above, we understand it that education is an essential requirement for the survival, growth and development of an individual in any society. If education is imparted in a proper way to fulfill the requirements of life, then the individual and the society survive in a better way. A properly imparted education perfectly shapes the personality of an individual making him aware about his and other's human rights. Real education never solves the problems for the person in a real life situation but it empowers him to solve his own life problems in a skillful manner. So in other words proper education promotes empowerment in a learner and enlightens him. In the contemporary social and educational scenario of India, imparting quality and meaningful education has various challenges and there is a need of removing these obstacles from the path. The basic problems those work like road blocks in imparting meaningful education are:

Language

Language as a medium of communication plays a crucial role in exchange of ideas and information. In Indian context, India is a multilingual country and at the same time there is not enough scope for the students in India to learn other languages than the mother tongue. Though the arrival of modern mass media has made Hindi popular in almost all the corners of the country but still the Indian students suffer from linguistic barriers till date. The popularization of English education and development of English as a window language at the world level has raised new challenges in front of the Indian educationists and students. Though speaking and writing of English are no more challenges to urban students but the same issue has remained as a challenge to the students of rural India which lacks from public schools and well trained teachers to impart English education in a better way. Both urban and rural students are equally talented but due to the constraint of English language, students from rural background suffer more than the urban students.

Lack of Communication Skills

Communication skills is one among the important requirements for imparting meaningful education among our students. Because having only knowledge is meaningless for a person if he/she is not able to express it properly at the time of need.

The Digital Divide

After the introduction of the digital technology in India a new form of class system has been introduced i.e. digitally literate and digitally illiterate. The digitally literate population has a better access to knowledge and information system where as the digitally illiterate population is still far away from it. In the digital class system, the digitally literate people are placed in the upper ladder whereas the digitally excluded people are getting placed at the lower ladder of the digital class system. They are getting deprived of the facilities of the digital society and the gap of inequality is becoming wider.

Banking concept of Education

Present educational system prevalent in our country is only based on the concept of retention of information and it is not much efficient to promote learning or developing life skills in a student. To speak in a better way if we analyze our present educational scenario we will find it that our educational system has a large amount of similarities with that of "Banking concept of education" conceptualized in Freirean pedagogy. In the banking concept of education, the teacher holds a key position and the student never becomes a part of the educational system which hinders learning. The process of learning is not participatory and it is completely authoritarian where the teacher imposes everything and the students work with the illusion of learning though they never become a part of the learning process. Thus the banking concept of education has the least scope for learning and at the same time, the banking concept of education being authoritarian and suppressive, kills the interest of students towards learning.

The Teaching Vs Preaching Debate

Teaching as a noble profession is involved with imparting knowledge within the students but in India most of the teachings are purely classroom based having no practical demonstration of the subjects. Again learning through observation and experimentation is too low in case of Indian teaching system. The classroom teaching in which the teacher goes on talking about subjects without creating realization among students also creates a problem for students to understand it and decreases the value of the education. Lack of practical demonstration and active participation between teacher and students is making the process of learning less interesting by changing the status of a teacher to a preacher.

Communicative Ecology and Traditional Knowledge System

Earlier while talking about communication, we have defined it as a process of human experience which plays a crucial role in information dissemination in the process of teaching. Culture as a part of the communicative ecology plays a crucial role to make communication process meaningful for imparting education. As India is a multicultural country so the communicative ecology is different from one place to another and it works as a big obstacle in imparting meaningful education. For example each society has its own model for educating its individuals and this traditional way of imparting knowledge has worked successfully for years among different communities. But before introducing any new approach to the learning system to make the process of learning more meaningful there should be a proper understanding of the traditional knowledge system and cultural values of society.

Thus, when Indian educational scenario is surrounded by such road blocks there is a need and necessity of strategic intervention to solve the problems of the educational system. Education should be designed in such a manner that it should bring critical consciousness among the students so that they can solve their problems by the knowledge they have acquired. In a better way following the Chinese proverb it can be said that "Give a man a fish and he eats for a day; help him learn how to fish, and he eats for life". Education should solve this purpose by igniting inner talents of the students. To satisfy the purpose of a meaningful education, it should be imparted in an attractive and fascinating manner. In an era when we are chatting about edutainment with slogans like "Karlo Duniya Muthi Main" and when android phones have started reaching to the vibrant new generation and the youth of this country have started loving technology the technology in itself is a solution to such problem.

With the repaid growth of technology we have reached to an era in which a sim card is cheaper than 1kilo rice, Mobile phones are sold with offers during festivals like dresses, our food is from Swiggy or Zomato, our travel depends on OLA or Uber, our clothes are from Myntra, our medicines are from netmed.com, our grocery shop is amazon, our fruit and vegetables are from bigbasket.com. our restaurant waiter or exam invigilator is a robot and along with Artificial intelligence and machine learning, we have started living in an era of man machine interface. Our relationships have gone shifted to virtual platforms and relationships in the physical environment are pushed to the corner. Our money has become the plastic money, our book has turned to the e-reader and our pen these days is the voice to text keyboard or the paint brush is the joystick. Thus the society surrounding us has changed, the cultural patterns have changed and our involvements with the social institutions have changed. Thus in such an environment of artificial intelligence and augmented reality or virtual reality we have started living in the environment of new educational and information technology and as a user centric and democratic platform, it has brought changes in the communicative behavior of its users. Concepts like edutainment and infotainment type have started becoming the reality of the day. Large amount of information is getting shared everyday through video based platforms to communicate with people in an effective manner to influence communication behaviors of people.

You Tube a powerful and popular platform

YouTube, the most popular video platform of internet was founded by Steve Chen, Chad Hurley, and Jawed Karim. All these three people were employees of PayPal. In its initial days, YouTube did not have much market recognition. On October 9, 2006, Google Inc. announced that it had acquired YouTube. Google's acquisition of YouTube changed

its fate. Later In 2010, it started free streaming of certain content. But in present scenario the market studies say that YouTube is the dominant provider of online video in most parts of world.it not only spreads entertainment content rather it also provides content on education and information in an attractive manner. Due to YouTube, the student community is capable of getting knowledge from top level professors of world. The YouTube as a powerful medium of modern communication has gone able to satisfy the communication needs of people in various manners and by character is quite different from the conventional media system. To speak in a nutshell, it is:

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- Mostly participatory and the rate of involvement of audience is very high.
- Audience has maximum opportunity to play the role of communicator and receiver.
- A liberal and democratic form of communication with ample opportunities for freedom of expression
- It is a new and attractive form of communication
- Creates a virtual world to provide a better satisfaction in communication.
- Communicator and respondent are known to each other.
- Individual members of the audience are mostly linked with a similar cultural background which makes the communication more effective.

The YouTube with above advantages and with its audio visual contents has become the potential new medium of today and it has started satisfying the uses and gratification perspective of people in a powerful manner. It has gone associated with our lives in such a manner that it has started influencing our lives in almost all spheres.

Economic Life and YouTube

The YouTube has become an industry itself today. The you tube channels are now new platforms of media business for creative people. YouTube is promoting financial literacy among people these days and it is become a new platform to promote business and has proved its effectiveness.

Cultural Life and YouTube

YouTube has become the new platform for cultural exchange. By YouTube we are able to know the cultures of people at different places. We are knowing about traditions and rituals associated with different societies. Folk dance, music and festivals are spreading among people through YouTube. Similarly the media and entertainment industry has also started using YouTube to highlight cultures of different people through their own programs. In fact new forms of culture are created and cultural diffusion has taken place through YouTube.

Social life and YouTube: Due to its wide presence YouTube has started influencing the social life in a powerful manner. In regular intervals contents in YouTube are highlighting issues of social interest and at the same time it is also talking about different discriminations and disparities prevailing in our society.

Educational Life and You Tube

YouTube has proved its usefulness through its audio visual contents. It has become a great source of knowledge distribution and information dissemination. Learning has gone easy due to video based explanations and demonstrations.

Legal life and YouTube

The YouTube in these days have started influencing the legal life of people because through YouTube different legal awareness forums have started creating videos for legal awareness among people and at the same different information relating to legal life have started influencing people.

Religious life and YouTube

May it be Durgapuja, Ramzan or Christmas these days the YouTube has become an important medium to spread the messages relating to religion. Advantages of using YouTube for Education: Anytime, Anywhere- YouTube as a tool

of communication is easily accessible and have no limitation of time and space. Information sharing through YouTube has gone popular all over the world. So lots of knowledge and information are getting shared by using YouTube by large mass of people. New ways of imparting education: YouTube has opened up new ways for teaching and learning. With the advent of YouTube, learning is no more restricted to printed books or materials rather list of learning materials have gone extended to video lectures and demonstrations starting from online study material. The open educational resources have started providing learning materials at free of cost. Low cost of Production: In most of the cases it is considered that production and distribution of YouTube based educational content involves more cost but as they have a wide reach and they are available in a potential forms with more possibilities of success, the production cost ultimately goes low. Considering the qualitative education aspect we can use YouTube in more easy and meaningful way.

Present scenario

In Indian scenario the number of instances of using YouTube for education have increased a lot and it has started reaching to all areas of life to bring changes. Looking towards the modern youth mindset telecom companies have started emphasizing more on data than calls. Thus these days the learners have started using YouTube in a more and more manner and if we will look into the modern learners, then we can realize it that with smartphones in their hands they have started gathering knowledge for their own need. Education has started becoming more and more interest oriented than compulsion. Thus, there is a necessity to understand the preferences and habits of the new age learners and their perceptions relating to YouTube as a learning platform.

Methodology and the Study

To understand the real scenario about learning preferences and perceptions of the new age learners relating to YouTube, a survey among the media students of Bhubaneswar from different media institutes located in Bhubaneswar. Media students were taken into consideration because they are the students who are non-technical but still they are the users. Methodology selected for the purpose of the study is survey, using questionnaires .Sampling technique used is convenient sampling. The study is conducted among 100 students. Bhubaneswar campus of the university is selected because in comparison to other 4 campuses of the university this campus has better internet connectivity. The study has used both primary and secondary data. Primary data is collected from respondents through interview and secondary data is collected from books. Magazines and Internet. The variables associated with the study are time and individual exposure to YouTube.

Use of the Medium

All of them have told that they use YouTube and all of them have also expressed that at different times they use YouTube for learning

Attractiveness of the medium

Responding to the question, whether YouTube is an attractive medium for learning, 93% of the users have told that YouTube is an interesting medium for learning and 7% of them have told that it is not an attractive medium of learning. While 60% of the respondents have told that learning through YouTube is more interesting than class room 33% have not become able to answer anything specific and 7% have told that classroom is more interesting

Learning preferences in YouTube platform

Talking about learning preferences in YouTube platform 73% of the learners have told that they prefer YouTube for learning, and 27% told other platforms or class room as their preferred resources. Similarly 40% prefer YouTube video lectures, 26% prefer to learn by joining social media groups, 20% prefer to contact the teacher directly and 14% prefer to contact other people. Talking about content type preference for learning, 51% prefer video lectures, 35% prefer the content depending upon the topic and 14% prefer text based content while learning. 48% of them expressed their dissatisfaction about advertisements in this video platform and 52% told that they do not worry

much about advertisements. 78% told that if they find a good channel matching to their need, they subscribe it and 22% told they dislike subscriptions. 53% told channel recommendations is good and 47% disagreed.

Learning and the nature of the medium

As nature of the medium also influences learning, that is why when asked about the quickness in getting solutions to questions, 93% have told that it is quick medium and 7% have told that they can't say anything properly. Answering to the question relating to the reliability of YouTube as a learning resource, 40% have told that the information available in YouTube are not reliable, 46% told sometimes the information are reliable and sometimes they are not and 14% told that YouTube is a reliable platform to provide correct information for learning.

Scope for improvement

While answering to the question relating to scope of improvement, 93% of the respondents have told that, there is still scope for it to develop as a better platform for learning and 7% disagreed to the fact.

Barriers

Answering to the question relating to barriers in using YouTube for learning, it was found from 35% of respondents that family restrictions are a barrier, 51% told connectivity, 14% told that advertisements and availability of large amount of resources. Talking about the content selection aspect and its' barriers 79% of the respondents told that information overload is an issue in content selection, similarly 14% expressed that they face problem due to their inability to comprehend the information to use it and 7% told they do not find proper information from YouTube to satisfy their learning purpose

CONCLUSION

From the above findings, it can be said that YouTube as a platform of learning has proved itself to be interesting and attractive for the learners of the new generation. Students have started accepting it as one of the prominent learning source due to attractive presentation formats of the content. However the users are also doubtful about the authenticity of the content in YouTube and barriers like internet connectivity or different restrictions are working like road blocks at the same time to establish YouTube as a better learning resource.

End Notes

An approach of educational system conceptualized by Brazilian Philosopher Paulo Freire

Critical consciousness is a stage in learning conceptualized by Brazilian Philosopher Paulo Freire in which there is a self-realization of the challenges and problems by learner by knowledge based empowerment of the self

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REVIEW ARTICLE

Big-Data Processing using Machine Learning: A Review

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ABSTRACT

With the advent of the computer and network technology, the size of data generated is increasing rapidly that lead to the growth of emerging applications like social network analysis, semantic Web analysis , which contains a variety of data(structured, semi structured and unstructured)to be processed . The term Big Data has emerged with new opportunities and challenges to deal with such massive amount of data. In modern digital world, the growing data size have resulted in newer ways of Big Data processing frameworks in order to get meaningful insights . For efficient data processing, Machine Learning based Big Data Processing framework has gained popularity among the various researchers. These type of new processing requirements have given a big boost to the development of new Machine Learning based methods for managing & processing them. In this paper it is presented a detailed review on machine learning characteristics in the context of Big Data and highlights the current scenario from different perspectives.

Keywords: big data, machine learning, big-data Processing

INTRODUCTION

Today in every field of study researchers are dealing with large scale datasets and lot of work is being carried out to better harness and process Big Data. The field of studies, that deals with processing of Big Data are like Engineering .Basic Sciences, Social Sciences, Bio-Medical Sciences, Applied Sciences and so on. Various factors that contribute the explosion of digital data like meteorological data, web-log files, sensor data, banking, growing social networks etc, because of which data volume is also growing exponentially . According to the Digital Universe Study, in 2011, 130 Exabyte of data were created and stored in 2005. The amount grew to 1,227 Exabyte in 2010 and was projected to grow at 45.2% to 7,910 Exabyte's in 2015[3]. by 2020, it is projected a third of the data in the digital universe (more than 13,000 Exabyte) will have Big Data value. Since the traditional tools and infrastructure do not work effectively

to handle these large, diverse and quickly generated data sets, there must be technology to capture, manage and process these unforeseen data, but still there are many challenges and issues which need to be tackled.

The advent of Machine learning has been an effective tool which holds tremendous potential in handling modern data challenges. Machine learning is the subset of Artificial Intelligence which has capacity to learn and is being widely used now-a-days in the number of applications like spam filtering, Alexa, Facebook etc. However, to date, there are relatively very few discussions that analyze deeply and systemically the new characteristics of machine learning in the context of big data and to provide various methods based on machine learning for dealing with big data. Remainder of this paper is organized as follows. Section II describes the related work in the literature. Section III presents the scope and relevance of the review on Big Data Processing using machine Learning and finally the summary of conclusion is presented in Section IV.

LITERATURE REVIEWS

because of the complexity of the structure of the big data, in recent years, most of the researchers are focusing on developing new framework for processing large scale data efficiently and to generate insight from it but with the existing technology, big-data processing has been a great challenges among the researchers, to address this issues, a large number of articles have been published by various researchers. for example,

In [1], Changqing Ji et al. presents the big data processing in the context of cloud computing. It discussed the key issues, including cloud storage and computing architecture, popular parallel processing framework, major applications and optimization of MapReduce.

In [2], Satoshi Tsuchiya et al. discussed on distributed data store and parallelization of complex event processing, which are basic technologies of Big Data processing.

In [3], C. L. Philip Chen et al. proposes several potential techniques to solve the Big-Data problem, including cloud computing, quantum computing and biological computing.

However, the above studies have focused on resource provisioning for the initial time.

In [4], Junfei Qiu et al. proposed a reference framework for processing big data based on machine learning techniques with the power of distributed storage and parallel computing.

In [5], Stefania Loredana NITA et al. discussed about big data, and have presented some characteristics of machine learning. It presented the most used machine learning techniques in big data, giving examples of applications for every described technique.

In [6], Junfei Qiu et al. discussed about the challenges of learning with big data and the corresponding possible solutions in recent researches. In addition, the connection of machine learning with modern signal processing technologies was analysed. It reviewed the machine learning techniques and highlight some promising learning methods in recent studies, such as representation learning, deep learning, distributed and parallel learning, transfer learning, active learning, and kernel-based learning.

In [7], Lidong Wang et al. presented some new methods and technology progress of machine learning in Big Data . it also discussed challenges of machine learning applications in Big Data.

In [8], Abdelladim Hadioui et al. gave an overview of the integration of learning analytics models into the phases of pre-processing of massive data in MOOCs, and it highlighted the advantages of integrating massive data into the process of developing learner profiles.

In [9], Roheet Bhatnagar et al. discussed the role of Machine Learning (ML) based algorithms and methods in Big Data Processing & Analytics (BDA). It also discussed key challenges associated with application of ML based approaches .

In [10], Shweta Mittal et al. discussed that since existing ML algorithms are not suitable for analysis of Big Data, ML algorithms needs to be optimized so that they can be effectively used for big data analytics. Optimization can be achieved by various Dimensionality Reduction techniques, Hashing, Data Cleaning, Sampling etc. Also, to minimize

the execution time, parallel programming techniques can be used. Hybrid machine learning algorithms may also be advantageous in case of big data and can be explored to obtain better results. In [11], Chao Shanga et al. reviewed the current status of research in the field of data analytics and machine learning oriented to data-driven monitoring, prediction, control and optimization and analysed the knowledge gaps to be filled in. Most of the above articles focuses on machine learning techniques that are good for processing structured data but they are lacking in processing semi-structured and unstructured data which requires massive computational efficiency and scalability to handle the huge data .Therefore more optimal techniques need to be designed that can process efficiently large volume of unstructured data in a real time manner .

BIG DATA PROCESSING USING MACHINE LEARNING

Big-Data

Big-Data is a term that refers to a huge volume of data that can not be processed or stored by any traditional data storage or processing units.

Big Data is categorized into three types, such as:

- Structured Data
- Semi-Structured Data
- Unstructured Data

Structured Data has a well-defined structure, it follows a consistent order and it is designed in such a way that it can be easily accessed and used by a person or a computer. Structured data is usually stored in well-defined columns in the Databases. Example: Database Management Systems (DBMS). Semi-Structured Data can be considered as another form of Structured Data. It inherits a few properties of Structured Data, but the major part of this kind of data fails to have a definite structure and also, it does not obey the formal structure of data models such as an RDBMS. Example:Comma Separated Values(CSV) File. Unstructured Data is a data which neither has a structure nor follow the formal structural rules of data models. It does not even have a consistent format and it found to be varying all the time.. Example: Audio Files, Images, video files, etc., According to Gartner definition "Big Data are high-volume, high-velocity and/or high-variety information assets that require new form of processing to enable enhanced decision making, insight discovery and process optimization[3].

Machine Learning

Machine learning is a field of study that gives computers the ability to learn without being explicitly programmed, aiming to understand computational mechanisms by which experience can lead to improved performance [4]. Most widely adopted machine learning methods are :

- Supervised learning.
- Unsupervised learning.
- Reinforcement learning.

Supervised learning : means it has a data set that includes the target values to predict. It receives a set of labelled data as inputs along with the desired outputs, and the algorithm learns by comparing its actual output with desired outputs to find errors and then modifies the model accordingly. It uses methods like classification, regression, prediction and gradient boosting to develop predictive model.

Classification problems ask the algorithm to predict a discrete value that can identify the input data as a member of a particular class or group. Regression problems are responsible for continuous data. Here, the input is sent to the machine for predicting the value according to previous instances. And the machine determines a function that would

map the pairs. If it is unable to provide accurate results, backward propagation is used to repeat the whole function until it receives satisfactory results.

Unsupervised learning: means it has a dataset which has no target to be predicted .It uses unlabelled data and find the hidden patterns or structure in data. Unsupervised learning is a type of self-organized learning that helps find previously unknown patterns in data set without pre-existing labels. Various methods includes k-means clustering , nearest-neighbour mapping, and self-organizing maps.

Reinforcement learning: In this method, the machine learn by it-self from its mistakes. Reinforcement learning is a type of learning that is based on interaction with the environment. It is often used for robotics, gaming because it discovers through trial and error. This type of learning has three primary components the learner or decision maker, the environment and actions [5].

Big-Data Processing using Machine Learning

Currently Big Data Processing has been a major focus area of research and many frameworks & techniques have been proposed by different researchers in recent past. But because of its very huge size of datasets with a great diversity of types it becomes difficult to process by using traditional data processing platform Big Data Analytics is helping organizations to improve business efficiency but then there are many challenges & issues associated with Big Data Processing & Analytics for each of the 5 Vs (Volume, Velocity, Variety Veracity, and Value)[9].

Machine learning is a rather efficient mathematics, based on statistical algorithms that can analyze large volume of diverse data sources. However, as the time for big data is coming, the collection of data sets is so large and complex that it is difficult to deal with using traditional data processing tools and models. As a result, some traditional machine learning techniques are unsuitable to this condition and cannot satisfy the requirements of real-time processing and storage for big data. Thus this needs us to explore some new methods with the power of distributed storage and parallel computing to analyze and deal with big data.

Currently several researches are focusing on Machine Learning based methods and their applications as an integral part of Big Data Processing, and also many new developments have happened in this direction..Qiu et al. [6] describes following future trends from different perspectives in ML based applications for Big Data Processing.

- Data Meaning Perspective: It implies as to how to make ML more intelligent to achieve context-awareness.
- Pattern Training Perspective: It implies how to avoid the over fitting during the process of training patterns.
- Technique Integration Perspective: It deals with integrating other related techniques with ML for Big Data
- Processing. Developing a composite, integrated and seamless platform for Big Data Processing have a great
- research potential.
- Privacy & Security Perspective: It provides a research direction for ensuring security and privacy in Big Data Processing using ML techniques.
- Realization and Application Perspective: How and where one must apply ML research in Big Data to gain optimal results. Applying and utilizing the developed ML techniques to real world problems carries huge potential as research area.

CONCLUSIONS

In this paper, an overview about big data is provided and summarized the types and characteristics of big data. Then a comparison of different machine learning techniques is made In order to highlight the use of techniques in the context of big data, The new features of machine learning with big data is then analyzed. Finally, several research

challenges and open issues are presented. This survey is intended to stimulate more interests in research and development of techniques based on machine learning for big data processing. In future it is planned to design a framework for processing big data based on machine learning techniques with the power of parallel processing in the cloud computing environment.

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Table:1. Some algorithms of machine learning and their Comparison

Algorithms	Types of Problems	Type of Data	Learning Types(Methods)	Data Processing Task	Real Time
Support vector machines, Neural Network, Random Forest, Hidden Markov Model, Bayesian networks Naïve Bayes	Regression and Classification	Labelled data	Supervised Learning	Classification and regression	Uses off-line analysis
K-means clustering, Gaussian mixture models, Self-organizing Maps, Apriori algorithm.	Association and Clustering	Un-Labelled Data	Unsupervised Learning	Clustering and prediction	uses Real Time Analysis of Data
Markov Decision Process, Q-Learning, R-Learning	Exploitation or Exploration	No-Predefined data	Reinforcement Learning	Decision Making	uses Real Time Analysis of Data

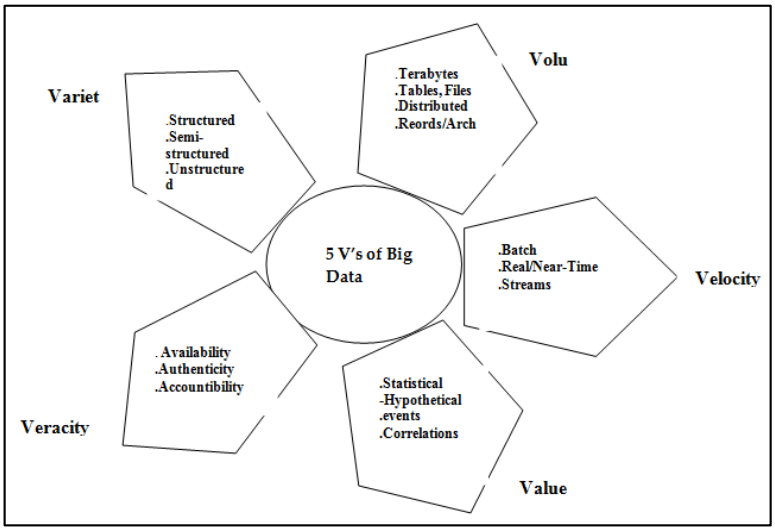

Fig. 1. 5V's ofbig data

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REVIEW ARTICLE

A Review on Potential Ethnomedicinal Plants used against Ocular Diseases

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ABSTRACT

This review summarizes the literature on medicinal plants used for the treatment of eye infection in the indigenous system of medicine. Medicinal plants have been used as traditional remedies for many diseases in different parts of the world from many years ago. In creating nations, natural material keeps on being utilized as the essential wellspring of meds in country territories. The eye is one of the most touchy and significant organs of the human body. Glaucoma, conjunctivitis, Cataract, Ocular inflammation, ocular allergy is common ocular diseases of human body. Among them cataract is the main cause of blindness in the world and in glaucoma disease damage the optic nerve. Glaucoma remains the primary driver of visual deficiency grown-up individuals more than 60 years of age. Conjunctivitis is the infection wherein the mucous layer shaped on the inward surface of the eyelid and causes eye bothered. Conjunctiva is a very thin, translucent membrane lining the anterior part of the sclera and inside of the eyelid. Due to many side effects of allopathic drugs, now a day's more numbers of herbal drugs are used for the treatment of eye diseases.

Keywords: Cataract, Glaucoma, Herbal drugs, Medicinal, Ocular disease

INTRODUCTION

Eyes are the organ of vision. They provide animals with vision, the ability to receive and process visual details. Without eye no one can be able to see anything. There are several natural mechanisms work for eyes to protect itself against various types of infection and diseases. For example "Eyelids and eye lashes protect the eyes from dust and any other type of foreign particles". Like that tear gland is present in eyes, from which tear secrets and keep the eye

surface moist. But sometimes due to some abnormal situation create in eyes or due to some foreign particle entry into the eye cause eye infection. After that severe situation created within eyes. A person faces several visual problems and unable to see anything surround him and slowly lost his vision. Eye infection normally caused by bacterial, fungal, viral and other type of micro- organism (1). To cure the eye infection people are using various type of chemical medicines and drugs. As a result, eye infection cure very soon but many side effects are shown and a person face eye sight problem in future. So that people must know the use of various plants for the cure of eye infection. Every plant has some medicinal properties, only people should know how to use them for a particular type of disease. Thus, medicinal plants are considered a good resource for drug development. By using herbal plant parts for various type of eye infection there is no side effect shown in future.

There are many more medicinal plants are present in our world. Among them half million plant species will be frequently used plants in future for drugs and yet many more medicinal plant's medicinal properties not known by people. But with the invention of "Modern medicine" people show disinterest towards herbal medicine and therefore there must be at last of the knowledge of traditional use of medicinal plants (2). Because people get medicine in market with low price and all the medicines are available in market. But to get herbal medicine people must know how to use the plant properly, which part of the plant used for a particular disease, how to make the drug from the plant part etc. So, they prefer chemical drugs first which are easily available in the market.
Various plant parts are used to treat sever diseases as well as wounds, dog and cat bites. It is also used to treat tetanus and to prevent rabies. However, some medicinal plants have major role against different eye infections. Several herbal drugs used against eye infection and there is no side effects (3).

Ethnobotany

"Ethnobotany is the study of a region's plants and their practical uses through the traditional knowledge of a local culture and people and this is also a part of human environmental science that defines the interface between people and plant and provides various types of substances which are needed for rural development based on sustainable yield from plants products" (4). Plants are normally found in open area seem to have potentials to provide options for rural livelihoods and biodiversity conservation for future use (5). These plants can contribute to poverty mitigation serving as subsistence "Safety nets" or low income "gap fillers" and these plants are useful for socio – economic, cultural, industrial and pharmaceutical uses, generating a lot of money annually to the world's economy (6). Ethnobotany is simply defined as the investigating plants used by societies in various parts of the world. It is usually focusing on the interaction of indigenous plants and local inhabitants (7).

The most ethnobotanical studies frequently report on the most important plant families based on a similar count of species used as a medicine (7-9). The university facilities have realized the necessity of introduction of new academic curriculum to train their students (10).Taking into consideration the above mentioned, one of the purposes of our project was to use the ethnobotanical survey as an educational tool for bachelor students. This study is a part of wider survey on current status of medicinal plant knowledge in Balasore district. Maximum people in the world population are uses traditional medicine, mainly medicinal plants for the cure of various diseases (11). The utilization of therapeutic plants in both a significant asset and a need and it likewise give essential medicinal services framework in creating nations (12).

Since long times ago plants have been essential source of defensive and therapeutic traditional remedy measures for humans and livestock. In India, such plants are utilized in treating pains, mucous discharge, wounded animals, constipation, gastric difficulties, headache, aching tongue in kids and fungal infection (13) The worth and information on restorative plants just notable by more established age who are gradually biting the dust with this information prompting the loss of significant data. The part of information and handling technique for unrefined medications are just accessible in rustic are of a specific network and keep up by these families and networks. At the same time youngsters show a lot of enthusiasm for formal instruction and once in a while get inspired by conventional information on restorative plants, therefore, quite a bit of these customary information remains and

announced and nearly getting lost. The viability of the vast majority of the natural medications has not been tried to verify the generally guaranteed rule in illness the board (14).Be that as it may, because of progress in way of life negatively affected keeping up conventional information on home grown cures; henceforth there is a risk of loss of this information. There is escalating decline of traditional medicine practitioners and consequently a loss in authentic traditional knowledge. (15).

Because of overexploitation and brushing of plant assets have just prompted a misfortune to the plant material accessible (16). Although there is much more progress occur in case of allopathic medicine, tribal people prefers herbal drugs for the cure of several diseases of mankind and pet animals. Total 80 percentage of the world population depend on herbal and traditional medicine (17). Because of better similarity, better social agreeableness with the human body and have lesser symptoms, these are oftentimes utilized in creating nations. There must be progress in tribal welfare for the development of ethnobotany. The world is outfitted with a rich abundance of restorative plants and these plants are a neighborhood legacy with worldwide significance. Plants have given a wellspring of advancement to novel medication compound which have made an enormous impact on human wellbeing and prosperity. They have various principles in that, they may turn into the base for the improvement of new medications and fill in as phytomedicine for the treatment of irresistible illnesses including the shrewd AIDS disease (18). The markers of medicinal plants have acquired some knowledge of the issues of some of these plants by interacting with the suppliers and end users. More authentic information on the curative properties of medicinal plants this can be obtained from practitioners of alternative medicine. Some of each practitioner's supply extracts packaged in various containers stating their curative properties but revealing little or no information on the plant materials contained therein.

Eye infection

The eye infection occurs when harmful foreign particles enter into the eyes and cause several disturbance inside the eyes, as a result a person face various eye side problems. It occurs when a potentially harmful micro-organisms like a fungus, a virus or a bacteria invade your eye ball or the area surrounding your eye. Simply the definition of eye infection is an infection of the sebaceous gland of the eyelid.
Various types of eye infections are described below:

Bacterial Eye Infection

When eye infection caused by various types of poisons bacteria that is called bacterial eye infection. "Among them *Streptococcus pneumonia, Haemophilus influenza, Staphylococcus aureus, Escherichia coli, Pseudomonas aeruginasa, Staphylococcus epidermidis, Bacillus cereus, Chlamydia trachoma* and *Neisseria gonorrhea"* (19). *C. Trichomatis* bacteria caused Trachoma which is the world's most dangerous eye infection which leads blindness and ocular morbidity (20). There are 146 million people suffering from trachoma eye infection. Burning, disturbance, tearing, and generally a mucopurulent or purulent release and so on are the manifestation of bacterial eye contamination. And also, in the morning eyelids are stuck together specially at the morning time. Usually bacterial eye infection is self-limiting. But if left untreated them develop into more serious eye side problem in eyes. It often improves in two to five days without treatment but can take two weeks to go away completely (21).

Fungal infection

There are various types of fungus by which eye infection caused, these are as *"Fusarium solani, Fusarium oxysporum, Aspergillus niger, Aspergillus flavus, Candida albicans* and *Penicillium notatum"* (22). The above-mentioned funguses are very dangerous. If someone infected may lose the vision capacity and become blind (22). The symptoms of fungal eye infections are eye pain, eye-redness, blurred vision, sensitivity to light, and excessive tearing eye discharge (23). After fungal spores go into the eye from an outer source, exogenous contagious endophthalmitis happens. When a blood stream infection spreads to one or both eyes, endogenous, endophthalmitis occurs. Fungal eye infection lasts seven to ten days. Contagious eye contaminations are amazingly uncommon, however they can be intense if

untreated. The most widely recognized path for somebody to build up a contagious eye contamination is because of an eye injury, especially if the injury was brought about by plant materials, for example, a stick or a thistle (24).

Viral Eye infections

When eye infection caused by various types of virus, it is called viral eye infection. Among them simplex virus-I, Adenovirus and Coxackievirus etc.(25). In developing country ocular infection caused by HSV-I virus which leads to blindness (26). HSV-I caused 95% of ocular harps. Usually viral conjunctivitis produces a watery discharge .Typically the infection starts from one eye and quickly spreads to other eye. No eye drops or ointments are effective against the common viruses that cause viral conjunctivitis (27).

Ocular disease

Glaucoma

"Glaucoma is a group of eye conditions that can cause blindness. With all types of glaucoma, the nerve connecting the eye to the brain is damaged, usually due to high eye pressure". Much of the time, glaucoma is brought about by higher-than-ordinary weight inside the eye-a condition called visual hypertension. Yet, some of the time glaucoma can happen in any event, when the weight inside the eye-called intraocular weight or "IOP" is typical (28). "Intra ocular pressure (IOP), ageing, family history, high myopia, systematic hypertension, cardio vascular disease, migraine headaches, peripheral vasospasm and prior nerve damage are some of the important recognised risk factors for glaucoma". Glutamate induced neurotoxicity, nitric oxide based damaged, disruption of neurotrophic factor transport and induced neuro- destruction is the leading possible factors of glaucoma. The liquid inside the eye, called fluid amusingness, as a rule finishes off your eye through a work like a channel. On the off chance that this channel gets blocked, fluid develops. Now and again, specialists don't have the foggiest idea what causes this blockage, yet it tends to be acquired importance it's passed from guardians to kids. Less basic reasons for glaucoma incorporate an unpolished or synthetic physical issue to your eyes. Serious eye disease blocked vein inside your eye and fiery conditions. The following types of glaucoma (29-31):

Open angle (Wide angle, chronic simple glaucoma)

"This is the most common type of glaucoma. Doctors are also called it wild angle glaucoma. The drain structure in your eye looks fine, but fluid does not flow out like it should". "It is probably a genetically predisposed degenerative disease affecting patency of the trabecular meshwork which is gradually lost past middle age".

Angle closure (narrow angle, acute congestive) Glaucoma

This is more common in Asia. "It also called acute or chronic angle- closure or narrow-angle glaucoma. Here eye does not drain like it should because the drain space between your iris and cornea becomes too narrow. As a consequence this can cause a sudden built up of pressure in your eye. It's also linked to farsightedness and cataracts, a clouding of the lens in your eye".

Secondary Glaucoma

"This is another type of glaucoma. When, a person suffering from cataracts or diabetes than this type of eye disease occurs due to increase pressure in eyes".

Pigmentary Glaucoma

In this case of eye infection tiny bits of pigment from eye iris, which is the colored part of our eye, get into the fluid inside eye and clog the drainage canals. A large portion of the individuals with open-edge glaucoma don't have any side effects. In the event that side effects do create, it's typically late in the illness with the goal that this sickness frequently called the (Sneak hoodlum of vision). For the most part, edge conclusion glaucoma indications come quicker and increasingly self-evident. Seeing coronas around lights, vision misfortune, redness in your eye, an eye that looks dim, upsets stomach or spewing and eye torment are the manifestations of glaucoma.

Cataract

"Cataract is a clouding of the normally clear lens of eye. people who are suffering from cataract, seeing through cloudy lenses is a bit like looking through a frosty or fogged-up window clouded vision caused by cataracts can make it more difficult to read, drive a car or see the expression on a friend's face". Early on most of cataracts develop slowly and don't disturb a person's eyesight but with the increase of the time it will eventually interfere with his vision. Cataract is a multifactorial disease and it is very important to identify the risk factors which cause cataract eye disease. These are various toxic factors, environmental, stressors and gene mutations.

Infection conjunctivitis

Conjunctivitis is a bothering or irritation of the conjunctiva, which covers the white piece of the eyeball. It very well may be brought about by sensitivities or bacterial or viral diseases. Conjunctivitis can be incredibly infectious and is spread by contact with eye emission from somebody who is tainted. On the off chance that conjunctivitis is brought about by a typical viral contamination and no different confusions happen, at that point your eyes should clear up inside a couple of days to about fourteen days. Be that as it may, when it is brought about by microorganisms, which even with treatment, for example, remedy anti-microbial eye drops can last as long as a month or more. By touching a unhygienic surface or by skin to skin contact it spreads from person to person. Symptoms include redness, itching and tearing of the eyes. It can also lead to discharge or crusting around the eyes.

Viral conjunctivitis

Viral conjunctivitis is an exceptionally infectious intense conjunctively contamination for the most part brought about by adenovirus. Manifestations incorporate disturbance, photophobia, and watery discharge.80% of instances of intense conjunctivitis are brought about by infections (32). 65% to 90% of instances of viral conjunctivitis are brought about by adenoviruses (33) and furthermore produce two kinds of basic clinical substances related to viral conjunctivitis. Pharyngo conjunctival fever and epidermic keratoconjunctivitis (34).

Bacterial conjunctivitis

Bacterial conjunctivitis is a typical kind of pink eye, brought about by microscopic organisms that taint the eye through different wellsprings of pollution i.e. abnormal proliferation of the native conjunctival flora, (35). Bacterial conjunctivitis is usually caused by "*Staphylococcus aureus, Streptococcus pneumonia, Haemophilus* species or less commonly, *Chlamydia trachomatis"*. The main symptoms of bacterial conjunctivitis include pinkness of the eyes, burning, itching sensation of grittiness or mild pain or discomfort in the eye, swollen and reddened eyelids. The course of the disease usually lasts 7 to 10 days (36).

CONCLUSION

This study has revealed that medicinal plants still play a very important and vital role in the provision of primary health care for the people. Just because of eye is the most important part of organ of human body. So, it should not be right to apply any chemical drugs for eye infection. In our surrounding many herbal drugs are present, which we can be used against different diseases particularly for eye infection and by using this there is no side effect cause. Thus people only should know the technique of using this herbal drug for particular disease.

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Table : 1. Types of cataract

Types of cataract	Causative Factor	Vulnerable People
Senile Cataract	"This cataract is caused due to the opacity of the eye lens by natural ageing process".	Elderly persons, mostly those over the age of 60 years.
Traumatic Cataract	"This cataract is caused due to some physical damaged to the eye lens capsule, such as that due to the entry	People working in hazardous condition such as welders and those in glass fornaces.

	of a difficult to remove foreign object".	
Complicated cataracts	"This cataract is the complication of some other chronic disease in the person".	Patience of diabetes and emphysema, asthma etc.
Congenital cataract	"This cataract is caused in infants if the mother had contracted German measles during pregnancy".	New born infants
Toxic cataracts	"This cataract is caused due to long term use of medicine or chemicals that are toxic to the eyes".	People using eye drops containing prednisone and cortisone for a long time. Also smokers as they inhale toxic fumes which affects the eye lenses.

Table:2.List of medicinal plants used against eye infection (37-44):

Sl. No.	Botanical Name	Local Name	Family	Parts Used	Uses in eye disease
1	*Acacia nilotica*	Kikar	Mimosaceae	Whole plant	For burring sensation in eyes
2	*Allium Sativum*	Garlic	Liliaceae	Bulb	Opthalmopathy, sore eyes
3	*Aloe vera*	China kalabanda	Liliaceae	Leaf	Ocular diseases
4	*Cadaba indica*	Patrika	Capparaceae	Leaf	Ocular diseases
5	*Camellia sinensis*	Green tea	Commelinaceae	Inflorescences	Conjunctivitis
6	*Capparis deciduas*	Kareera	Capparidaceae	Leaf	Corneal opacity
7	*Capsicum annum*	Capsicum	Solanaceae	Seed	Ocular diseases
8	*Carissa opaca*	Granda	Apyocynaceae	Stem, leaf, Fruit	Ocular diseases
9	*Cassia absus*	pig's senna	Caesalpiniaceae	Leaf, seeds	Ocular diseases, strengthens eye sight
10	*Cassia auriculata*	Avaram Senna	Caesalpiniaceae	Seed	Eye infections
11	*Cassia italica*	Balibali	Caesalpiniaceae	Leaf	Ocular diseases
12	*Cassia obtusifolia*	Juemingzi	Leguminosae	Seed	Eye infection
13	*Cassia occidentalis*	Peedachennangi	Caesalpiniaceae	Leaf	Sore eyes
14	*Cassia tora*	Tailancha	Caesalpiniaceae	Leaf, seed	Ocular diseases
15	*Celosia argentea*	Guruguaku	Amaranthaceae	Seed, leaf	Blurred vision, eye inflammation
16	*Centaurea calcitrapa.*	Red starthistle	Asteraceae	Whole plant	Ocular diseases
17	*Chenopodium album*	Bathu Saag	Chenopodiaceae	Whole plant	Ocular diseases
18	*Clitoria ternatea*	Blue pea vine	Fabaceae	Root, Leaf	Eye inflammation
19	*Costus afer*	Spiral ginger	Costaceae	Rhizome, Leaf	Ocular diseases
20	*Crepis cameroonian*	Hawk's-beard	Asteraceae	Leaf	Ocular infections
21	*Curcuma longa*	Turmeric	Zingiberaceae	Rhizome	Ocular diseases

22	*Curcurbita pepo*	Pumpkin	Cucurbitaceae	Fruit	Good for eyes
23	*Cyperus nevieus*	Deela	Cyperaceae	Root	Eye sore
24	*Cyperus rotundus*	Mustaka	Cyperaceae	Rhizome	Ocular diseases
25	*Datura metel*	Dhutra	Solanaceae	Leaf, root, Seed	To enlarge pupil in eye
26	*Datura stramonium*	Datura	Solanaceae	Seed	Iritis
27	*Daucus carota*	Carrot	Umbelliferae	Seed	Eye sight, glaucoma
28	*Desmodiumincanum*	Creeping Beggarweed	Fabaceae	Bark	Eye problem
29	*Euphorbia hirta*	Dodhi	Euphorbiaceae	Leaves, Inflorescence	Redness of eyes, remove foreign body from eyes
30	*Ficus benghalensis*	Bargad	Moraceae	Latex, stem	Eye pain
31	*Flacourtia indica*	Rakatsonk	Flacourtiaceae	Leaf	Conjunctivitis
32	*Foeniculum vulgare*	Fennel	Apiaceae	Leaf, flower	Conjunctivitis
33	*Fuerstia africana*	Birirwobsot	Labiatae	Leaf	Eye problems
34	*Fumaria officinalis*	Paptra	Fumariaceae	Leaf, stem, Flower	Conjunctivitis
35	*Ginkgo biloba*	Maidenhair Tree	Ginkgoaceae	Leaf	Retinal vein occlusion, glaucoma
36	*Heliotropiumindicum*	Hatisuri	Boraginaceae	Leaf, root	Conjunctivitis
37	*Iris germanica.*	Lirio	Iridaceae	Flower	Conjunctivitis
38	*Jasminum arborescens*	Jasmine	Oleaceae	Leaf	Eye problems
39	*Jasminum officinale*	Chameli	Oleaceae	Root	Eye problems
40	*Jatropha curcas*	Adaviamudamu	Euphorbiaceae	Latex	Ocular infections
41	*Jatropha gossypifolia*	Ratanjot	Euphorbiaceae	Latex	Corneal opacity increase eye sight
42	*Juniperus excelsa*	Apurs	Cupressaceae	Seed	Ocular diseases
43	*Kalanchoe densiflora*	Air Plant	Crassulaceae	Leaf	Conjunctivitis
44	*Kalanchoe pinnata*	Air Plant	Crassulaceae	Leaf	Ocular diseases
45	*Lepidium sativum*	Zachik	Brassicaceae	Seed	Eye problems
46	*Leucas aspera*	Kubi	Labiatae	Leaf	Ocular diseases
47	*Leucas aspera*	Thummi	Lamiaceae	Leaf	Ocular infections
48	*Lippia nodiflora*	Poduthazhai	Verbenaceae	Whole plant	Ocular diseases
49	*Luffa acutangula*	Ridged Gourd	Cucurbitaceae	Leaf	Granular conjunctivitis, prevent excessive meihomian secretion
50	*Lygodium salcifolium*	Chumng	Lygodiaceae	Leaf	Pain in the eyes and night blindness
51	*Madhuca indica*	Madhuka	Sapotaceae	Flower	Ocular diseases
52	*Mangifera indica*	Mango	Anarcardiaceae	Unripe fruit	Blindness
53	*Manihot esculenta*	Bankye	Euphorbiaceae	Leaf, root	Ocular diseases

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REVIEW ARTICLE

Review on Allelopathy: A Natural Way Towards Wild Plant Management

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ABSTRACT

India is the land of biodiversity. Nature acts as a good providing source for both human being and animal kingdom. Allelopathy has been known and utilized in agribusiness since the antiquated occasions. Allelopathy is a typical natural marvel by which one life form produces biochemicals that impact the development endurance advancement and propagation of different organisms. These biochemicals are known as allelochemicals and have helpful or hindering consequences for target living beings. To guarantee practical farming improvement it is imperative to abuse development frameworks that exploit the stimulatory/inhibitory impact of allelopathic plants to direct plant development and advancement and to keep away from allelopathic autotoxicity.

Keywords: Agribusiness, Allelopathy, Biochemicals, Farming, Plants

INTRODUCTION

"Allelopathy is a part of chemical ecology which concerned with the effects of chemicals that is produced by plants on the growth; it helps for the development and distribution of other plants in natural communities" (Einhelling, 1995). "The term allelopathy was first introduced by Molish in 1937 to show all of the effects that result from biochemical substance which move from one plant to another" (Molish, 1937). The collaboration of allelopathic is one of the critical elements give to species dispersion and a huge amount inside plant networks and it additionally assume significant job in the achievement of intrusive plants (Chou, 1999; Mallick and Mohan, 2003; Inderjit et al., 1997). Plant discharged a few synthetic substances and executing allelopathic impact are named as allelochemicals or allelochemics and allelochemicals are the optional plant metabolites, that is biosynthetically gotten from the essential

metabolites of the plant (Torres et al., 1996).After some year later, the algae, fungi and various microorganisms are accepted as targets of allelochemicals.

This form was polished by Rice (1984) to state that "any direct or indirect harmful or beneficial effect by one plant (including microorganisms) on another through production of chemical compounds that escape into the environment" (Rice, 1984). Allelochemicals contains several type of chemical families and they are divided into following 14 categories, which is based on chemical similarities like: "water- soluble organic acids, straight-chain alcohols, aliphatic aldehydes, and ketones; simple unsaturated lactones; long- chain fatty acids and polyacetylenes; benzoquinone, anthraquinone and complex quinines; simple phenols, benzoic acid and its derivatives; coumarin; flavonoids; tannins; terpenoids and steroids; amino acids and peptides; alkaloids and cyanohydrins; sulphide and glucosinolates; and purines and nucleosides".

Allelochemicals can direct or restrain plant germination and development, and permit the advancement of yields with low phytotoxic buildup sums in water and soil, in this manner encouraging waste water treatment and reusing (Macias et al., 2003). These were a suitable substitute for manufactured herbicides in light of the fact that allelochemicals don't have harmful impacts, in spite of the fact that the viability and disposition of numerous allelochemicals are constrained (Bhadoria, 2011). Exploration of allelopathy prompts the motivation behind application which watched allelopathic impacts on farming creation, reduction of the contribution of substance pesticides and subsequent natural contamination and giving viable strategies to the practical improvement of horticultural creation and environmental frameworks (Macias et al., 2003). In agribusiness, the allelopathic crops are utilized as of late being acknowledged, e.g., as segments of yield turn, for intercropping, as spread harvests or as green excrement (Cheema and Khaliq, 2000; Sing et al., 1999; Irshad and Cheema, 2004; Iqbal et al., 2007).

There were several competitions occurring in among cultivated crops and their nearest plants (Inderjit and moral, 1997; Xian et al., 2005). Allelopathy contain a chemical mechanism which give an benefit for challenging for inadequate resource in plants (Singh et al., 1999). In fields the weeds were controlled by using crop allelopathy, to alleviate allelopathic autotoxicity and reduce inhibitory influence among allelopathic crops (Iqbal et al., 2007; Farooq et al., 2011a). By using crop rotation and intercropping systems, biomass production and weed population density can be significantly reduced (Liebman and Dyck,1993). So the allelopathic nature of crops must be advised in intercropping, crop rotation and stalk mulching (Xuan et al., 2005). Allelopathic plants used as land wrap genus, that provides an ecological forthcoming option (Dhima et al., 2006). In the South-eastern region of Brazil, the fruit peels of coffee (*Coffea arabica*), that contain allelochemicals like: caffeine, phenols and flavonoids, which is used as an organic amendment in agricultural practice to control weeds (Silva et al., 2013). From allelopathic plant, there are some natural herbicides or plant development inhibitors are produced to restrain weed development in fields (Guillon, 2003).

ABROAD
CHINA

The primary distribution presenting the word allelopathy in the Chinese writing of this exploration is distributed in the Chinese with the monograph "Allelopathy and its application" (Kong and Hu, 2001). From Chinese germplasm collections the allelopathic rice and wheat admittances were appraised and screened (Kong et al. 2002; Zuo et al. 2005). A new method has been developed using chemical fingerprinting to evaluate allelopathic crop admittances and individual plants in a non-destructive manner (Kong et al. 2002). At early development arranges, the root exudates from *A. hypogaea*, before the arrangement of root knobs, advanced development of rice, maize, radish and rye grass. This is by all accounts because of the root exudates of *A. hypogaea* triacontanol is found at 1-3 leaf development stage, which effectsly affects the plant development (Hu and Kong, 2002). The growing allelopathic wheat varieties considerably decreased the weed biomass in several corn crops and also reduce weed infestation in

the wheat field which is demonstrated in the field experiments (Ma et al. 1996). The restraint of all wheat genotypes, barring *Secale cereale* L., had allelopathic impacts; brought about by the wheat genotypes expanded as their genome changed from 2n to 4n to 6n (Zuo et al. 2005). The beneficial outcome on the creation allelochemicals, because of the nearness of *E. Crus-galli* , herbicide stress, bright light, jasmonic corrosive application and furthermore substantial metal harm (Kong et al. 2004a; Zhao et al. 2005).A cross between Indica rice assortment Zhong 156 Gumei 2 was attempted to outline quality liable for the allelopathic impact on farm grass, which is gotten from a populace of 134 recombinant ingrained lines (RILS) (Xu et al. 2003).

In China, the allelopathy of different sorts of weeds, particularly extraordinary weeds, have been examined, that is *Ageratum conyzoides* L. Has been concentrated in detail (Kong et al. 2004b). The weeds were effectively suppressed and controlled other insect pests by the intercropping of *A. conyzoides* in citrus orchards. Through the ageratochromene and other allelochemicals released into soil by *A.conyzoides*, the weed and soil pathogenic fungi were effectively suppressed (Kong et al. 2004c). *C.equisetifolia* released some allelochemicals, which inhibited root growth of *C. equisetifolia* seedling and that is showed by research (Deng et al., 1996). From *C. Lanceolata* litter and soil in *C. Lanceolata* woods, a few allelochemicals were confined and they fundamentally repressed the ghowth of *C. Lanceolata* seedlings and in this way influenced the recovery procedure (Chen et al., 2005). In several aquatic ecosystems, the algal and macrophytes were antagonistic to each other (Xian et al. 2005). Under different environmental conditions the allelopathy and competition between *A. tatarinowii* and algae were investigated (Ye et al., 1999).

PAKISTAN

Prof. H.M. Naqvi began researching the allelopathic capability of many grass species while working at the University of Peshawar in Pakistan. Dr. Farrukh Hussain has accomplished the work in certain different species and discovered outcomes especially from buffel grass (*Cenchrus ciliaris*); which buffelgrass restrained the germination and shoot development of foxtail millet (Setaria italic), cattail millet (*Pennisetum americanum*), lettuce (*Lactuca sativa*) and mustard (*Brassica campestris*), when Naqvi moved to the US in 1975 (Hussain and Anjum, 1981). Allelopathic impacts of millet, sorghum and pear were changed by manure and customary culturing (Arshad 1995). Two national ventures have finished by Cheema and his partners at various areas in Punjab, Pakistan. Acombination of allelopathic crops removes (brassica, sunflower, sorghum) can diminish the herbicides utilization by 50 to 75% in field harvests, for example, maize, rice, wheat and cotton were finished up by them (Irshad and Cheema, 2004; Iqbal and Cheema 2007; Jamil et al. 2009). Water concentrate of mulberry (Morus alba) joins with the sunflower and sorghum which repressed weeds in wheat fields (Jamil et al 2009). The brassica dust is contain some sign of promotive impacts and brassinolide compound is distinguished (Grove et al. 1979).

Several reports state that certain growth process as germination of different test species were stimulate by allelopathic extracts at lower concentration (Cheema 1988; Randhawa et al. 2002). It was considered that two splash of canola and moringa blend showered at 40 and 30 DAS, which expanded blend grain yield by 83% (Hussain, 2010). On the planet over, there is an ever-expanding push for naturally delivered materials. There has been an attention on plant-inferred wares as an eco-accommodating methodology which can the substitute herbicide for weed the executives during last two decads (Cheema et al., 1997).

RUSSIA

Red root amaranth (*Amaranthus retroflexus* L.) is distributed world wide, which is a serious destructive weed, especially in garden, orchards, farmland, wasteland and the roadside. Due to its large amount of seed and strong flexibility its control is very hard. The growth of several crops can seriously affected by red root amaranth and it causes great loss to agricultural production (Costea et al., 2004; Li et al., 2004). In North America an exotic invasive

plant is found that is "*Acroptilon repens* (L.) DC (Russian knapweed; formely *Centaurea repens*), a perennial herbaceous plant belong to family Asteraceae, which suspected to be allelopathic" (Fletcher and Renny, 1963). Russian knap weed contain phytochemicals which is harmful to other plants (Stermitz et al., 2003). In North America it is a persistent weed problem, because of its extremely reasonable character and broad environmental flexibility (Goslee et al., 2001).

These monocultures have been allocated to various variables, similar to adaption to unsettling influence, and it contains a broad root framework, and through the creation of natural allelopathic synthetics it obstruction with neighboring plants (Selleck 1964; Goslee et al. 2001). The creation of harmful natural-synthetic concoctions are completed by the impedance between plants (Harper 1977). The term "elemental allelopathy" is defined as the intervention mediated throughout the addition and concentration of non-living elements (Boyd and Martens 1998). "Biochemical allelopathy has been studied by speculation and assumptions" (Inderjit and Del Moral 1997). There is a cool-season bunchgrass called *P. Soicata* which is a less competitor with many invasive weeds. Also *P. Juncea* is a cool season bunchgrass which is inhibited by *A. repens* and that was expected to be tolerant of elevated Zn levels (Bottoms and Whitson 1998; Monsen et al. 2004).Within an *A. repens* monoculture, high Zn riched soil was collected from the top 7.5 cm layer (Bottoms 2001).

INDIA

The term "allelopathy is defined as some direct and indirect effect of one plant on another through the production of chemicals" (Rizvi and Rizivi, 1999). Generally, the allelopathic compounds present in natural plant communities, these are contain a mechanism by which weeds interfere with crop growth (Bell and Koeppe, 1972).The germination and growth of crops are affected by several weed species due to its toxicity. There are some major problems in the rice production field to manage the weed, which is a challenge for the rice farmers. In China, the annual loss of rice production is 10 million metric tons due to weed competition (Zhang, 2001).

Holm et al. Reported that *Cyperus iria* L. Is one of the most common weeds of rice in Srilanka, India and Philippines. Association between *C. Esculentus* and *P. hysterophorus* that show a huge impact on radical length, germination rate, plumule length, new weight, and dry load of seeds. "Any process involving secondary metabolites produced by plants, microorganism, viruses and fungi that influence the growth and gdevelopment of agricultural and biological systems, including positive and negative effects", this statement was defined by the International Allelopathy Society in 1996 (Rice, 1984). From plants several chemicals released and imposing allelopathic influences are known as allelochemicals or allelochemics (Torres et al., 1996). The growth, germination and development of severalplants are affected when they exposed to allelochemicals (Inderjit and Moral, 1997). These compounds are also known as 'natural herbicides'. "The allelopathic effect of hydroalcoholic extract of ashwagandha (*Withania somnifera*) can used for the germination and radical growth of *C. arietinum* and *T. aestivum"* (Macias, 1995).The radical growth and percentage of germination were recorded, which monitor the allelopathic behaviour (Kruse et al., 2000).

Some invasive plant released chemicals which discourage growth of native plants is known as allelopathy (Heirro and Callaway, 2003). Due to allelopathy, Lantana disturbs progression, decline biodiversity, and can lessen life of local plants. The leaf concentrates and leachate of Lantana, that decline the seed feasibility, germination, speed of germination and seedling development limit of *Mimosa* seeds (Maiti et al., 2008)."The aqueous leaf extracts of *L.camara* at different concentrations, that shows inhibitory effect on root, shoot elongation and germination of several food crops like *Cicer arietinum*, *Brassica juncea*, *Phaseolus mungo*, *Cucumis sativus*, *Vigna unguiculata* and *Raphanus sativus*" (Ahmed et al., 1972). The germination of spores of the liverwort *Asterella angusta* was inhibited by leaf extract of *L. Camara* which exhibit a potential against other plants (Kothari and Chaudhary, 2001). The growth of *Parthenium hysterophorus* was inhibited by high concentration of leaf extract of Lantana in flowering stage (Mishra, 2014).

ODISHA

An annual herb like Hyptis, which aggressive nature and that contains several chemicals like phenol, saponin, tannin, carbohydrates, alkaloids, steroids and flavonoid (Mudgal et al., 1997). The leaf extract of *Eucalyptus urophylla*, which inhibit the, root initiation, number of roots and root length of hypocotyls of mung bean and pea (Huang et al., 1997). The aqueous extract of *Hyptis suaveolens* showing the weedicidal effect, so that it contain allelopathic potential (Rao et al., 1987).

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RESEARCH ARTICLE

Transformation in Effective Inclusive Education and Personalized Learning by Integrating IoT Technologies

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ABSTRACT

The Internet of Things (IoT) technologies offer a great scope for educational system to improve learning skill and improve the complete educational operations. IoT in education (IoET) allows transforming traditional education system into adaptable, scalable and effective e-learning in a platform for interacting educational objects. This paper analyzes the manners to achieve enhanced educational practices using IoT that enables the customization of education to give every learner access to their needs and capabilities thus making personalize learning. Besides this, it has investigated the potential of IoT in education for students with disabilities to maintain adaptive and sustainable educational environment through IoT-enabled assistive technology and establish an effective inclusive education system.The objective of this paper is to explore the potential of IoT technologies that can transform effectively in inclusive education and personalized learning.

Keywords: Inclusive education,IoT, IoET, ICT,personalized learning,smart learning.

INTRODUCTION

Inclusive education is the practice of addressing the diversified needs of learners through increasing participation in learning, cultures and communities [1]. The objective is that the entire education system will enable learning atmospheres and each student has an opportunity to succeed [2].Artificial intelligence (AI) offers remarkable potential for use in education. Today's educational institutions intercept many problems like disengaged students, high dropout rates, and the ineffectiveness of a traditional "one-size-fits-all" approach to education [3]. The human has improved the quality in life by making innovative opportunities, services, mechanisms and professional models due to the technological developments. People can interact to the environment with the help of these advances in

different ways and capabilities. Internet is one such technology that redefines the world by interconnection of people and things, referred to as Internet of Things (IoT). Now there is atransformation from Internet of computers into the Internet of people, known as Web 2.0 [4]. An innovative technological trend in the Internet world is the IoT which enables connectivity for anything and for anyone to be interconnected around the globe at anytime and anywhere using any communication technologies to achieve the goal of intelligent detecting, monitoring and handling things. The IoT has the technical properties that enable the advanced services by interconnecting things based on interoperable ICTs. Based on this idea number of devices and things are connected to the Internet, each providing information and services. This technology provides an opportunity for expanding the communication between human to human (H2H), human to things (H2T) or things to things (T2T) for intelligent decision making by interacting with each other [5]. This paper presents a unique Information and Communication Technology (ICT) viz. IoT that is integrated with education for the improvement in personalized learning and inclusive education by addressing learning challenges for disabilities.

Exploring of IoT in Education

IoT in education provides scopes for upgrading the education system in terms of teaching and learning, classroom monitoring, and attendance monitoring automation, student physical and mental health,school security and personalized learning. Integrating IoT in education is referred to as Internet of Educational Things (IoET)that interconnects not only computers, tablets and smartphones, but also it allows connectingevery other educational things to the Internet. Thus it completely changes the traditional model of education [6].IoT is a network of a diversity of connected educational things. Technology in education has played animportant role in integrating and educating the students.The learning activities and the corresponding learning outcomes in the educational institutions are enhanced with the establishment of IoT by providing richer learning tools and pedagogyand gaining real-time interaction with student performance.

The istitutions haveprospect to lead the technical growth and the innovations models for the IoT and has the potential to address the issues like privacy, trust, protection and security associated to the IoT[7]. A Smart educational campus consists of smart IoT-based classroom, lab, sensors, smart educational things, data analytics, cloud computing, artificial intelligence and RFID technology [8]. AnIoT based smart learning system with its important components is shown in figure 1. Educational environment is equipped with advanced learning aids based on smart things such as intelligent sensors with cameras, microphones. IoT in a classroom can help to provide a better teaching and learning environment [9]. The cloud computing system helps to control and manage the activities in the classroom. Smart devices have made it possible for a teacher to adopt dynamic nature of the students. Thus incorporating IoT devices in teaching and learning is a recent trend which provides an innovative approach in educational management.

Role of IoT inPersonalized Learning

In personalized learning, every student will avail unique educational approach based on specific abilities and requirements. The teachers will be provided useful information about their students' learning abilities, and progress, and deliver suggestions to customize teaching methods [10]. The learners have diverse abilities and unique ways to respond learning opportunities. The institutions face massive challenges in community education system to equitably recognize these differences and develop learning approaches for all learners to achieve satisfactorily. Creating personalized learning situations for each learner we can increase equity by providing every learner what they need to be successful irrespective of language, culture, socio-economic background, competition, ethnicity, physical and mental abilities. Thus there is a need of personalized learning [7].

Personalized learning provides an approach that equitably supports educators' efforts to empower learners as individuals and thus it incorporates differentiation and individualization. Adaptive learning technology can be used with the use of technology and tools to assign digital resources to learners based on their unique needs[11]. The basic components of a personalized learning are represented in the figure 2.The process could include whole-class in small-group activities and learners engaged in digital learning activities with technology used that can measure performance continuously in real time.The use of technology enables the teachers to tailor instruction to provide targeted attention to learners who are struggling. IoT enables the customization of education to give every student access their needs. Collecting data about student performance during lessons as well as tests enables the educators to personalize learning as per their interest as well as capabilities [12]. Artificial intelligence (AI) offers high potential for the application in education. Big data analytics and artificial intelligence can provide personalized learning experiences which in turn help to resolve many challenges [13].It gives teachers the useful information about students' learning abilities and provide suggestions to customize their teaching methods to individual needs[14].

Assistive Technology for Inclusion of students with Disabilities

Inclusion of persons with disabilities has been a challenge always. Certain progress is being made in improving inclusion through policies and technologies. Assistive technology is any device or software that is used to improve the functional capabilities of persons with disabilities like visual impairment, hearing impairment, speech impairments, physical and cognitive impairment etc.[15]. Assistive technology is designed to help students who have learning disabilities and allow them to function within the classroom.

Assistive devices are suitable for students with visual impairment or low vision to assist in effective learning. Software can allow users with visual impairment to read documents on a standard scanner with optical character recognition and read using speech synthesis. Text-to-speech software can help the user in adjusting the volume, pitch and speed of reading [16]. Students with low vision not able read small text mayuse large key labels, special equipment for display adjustment, computer-generated enlarged symbols, text and graphics on the monitor. Modifying the color of the monitor or altering the foreground and background colors can help to enhance access and readability for the students having problem to distinguish colors. An RFID-based assistive device application is the navigation system. Visually impaired people require specialized Human Machine Interface (HMI) to control home-based equipment. Specialized zooming devices allow people with low vision to control the home setting[17].

Assistive devices that are suitable for students with hearing and speech impairments can aid in efficient learning[18]. Advanced speech synthesizers act as alternative tool for students who cannot interconnect vocally. Speech recognition software can change a spoken message into a text document that allows the hearing impaired students to read easily.Deaf or hearing impaired people require specialized HMI touch screens to access graphical information and read text. The assistive devices designed for the hearing impaired aresensors and RFID-based devices [19]. A number of assistive technology devices that helps people with physical and cognitive impairments used for learning disabilities are eye gaze trackers, variable speed recorders, speech synthesizer**,**videotaped social skills, math simulations**, a**bbreviation expanders, OCR, FM listening systems, speech-recognition software and word-prediction platforms [20].

IoT technologies and applications have the potential to help people with disabilities for providing education in a better way and accelerate development of assistive technologies. Education for students with disabilities could be improved through the provision of IoT as the assistive technology.IoT and wearables have enormous potential to help the people with disabilities in learning [21]. The basic structure of an IoT-enabled learning for disabilities is represented in figure 3. Many assistive devices are built using artificial intelligence (AI) technologies, including real time speech-to-text transcription and visual recognition tools. Its use in the education space has the potential to help students with disabilities overcoming disability-related learning challenges making the tertiary learning environment [22].With IoTdevelopment, the advances of brain gate technology and brain-computer interfaces made possible the development of models such as brain-controlled prosthetic devices, keyboards and computer games. BCI

technologies can be transformed into real-world applications such as communication and control, motor substitution and entertainment etc[23,24].The World Wide Web could help address various issues relating to the needs of people with disabilities by providing a universal interface to IoT as it does for the traditional internet referred to as Web of Things (WoT) [25].

The key challenges in Integration of IoETcomprise **s**ecurity, mobility, interoperability, scalability. network bandwidth, web analytics, teacher training and cost etc. The growth of integrating IoT in education is increasing and it will have a great impact in future education. It will have more integration of IoT with AI for efficient personalized learning and helps in development of advanced adaptive assistive tools to address learning challenges for disabilities.

CONCLUSION

The IoT in education helps to develop an efficient e-learning farme work to predict the educational needs of the students from the inter connected objects andenables the customization of education to provide every student access to their needs that can regulate their preparation actively and passively enabling the educators to personalize learning as per their needs and capabilities. Besides this, education for students with disabilities could be improved through the utility of IoT-enabled assistive technology. Its use in the education space has the potential to help students with disabilities by overcoming the disability-related learning challenges and enable for effective inclusive education. IoT technology has opened the door ways for innovative ideas in the field of education through artificial intelligence for improvement both students and teachers. Alongside technology, enhanced IoT-supported educational environment demands a higher degree of research in designing IoT-based intelligent teaching-learning platforms.

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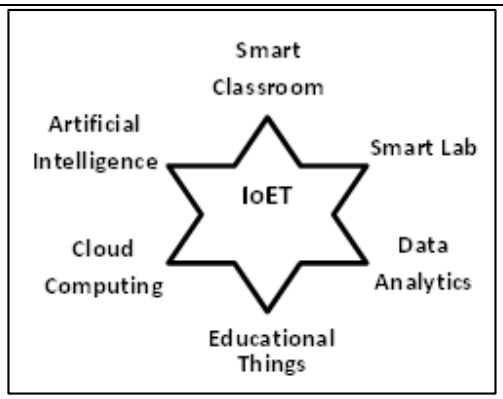

Figure 1: IoT-based Smart Learning

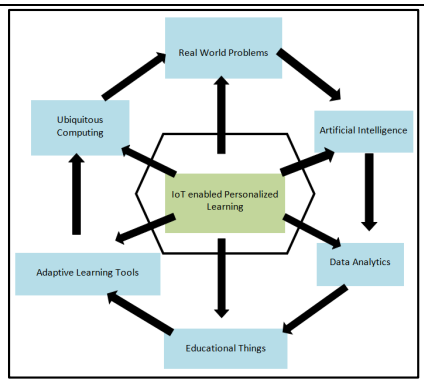

Figure 2: IoT enabled Personalized Learning

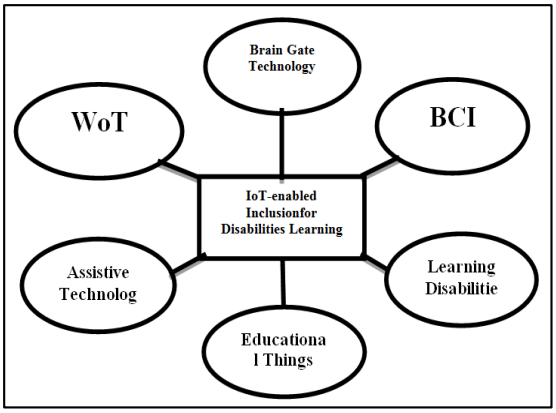

Figure 3: IoT-enabled Assistive Technology

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RESEARCH ARTICLE

Grain Biology of Selected Rice Landraces of Southern Odisha

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ABSTRACT

The present work is an attempt to study the grain biology of selected rice landraces of Southern Odisha to recommend the best varieties suitable for cultivation in different agro climatic zones for which 10 rice landraces cultivated using traditional methods and unique in their morphological characters of shape, size and colour were selected. Most of these rice landraces are grown in pristine habitats by a small group of marginal farmers residing in the tribal belts of Southern Odisha who serve as the custodians for these races. The 10 rice landraces selected for the present study are available in the Jeypore tract of undivided Koraput district and are known by their local names as Tiki chudi, Asamchudi, Baunsidubraj, Deulabhoga, Kanakchudi, Muktabali, Kalamalli, Kandulakathi, Dudhamani and Sapuri respectively. The studies carried out with reference to grain biology include the determination of the percentage of seed germination and seedling establishment, changes in the shoot and root length of seedlings, determination of total biomass in terms of their fresh and dry weights, photosynthetic efficiency and changes in gross photosynthetic and respiration rates. The results of the study indicate an immediate attention to conserve the gene pool for restoring the biodiversity of rice landraces.

Key words: Landraces, custodian, germination, biomass, photosynthetic, biodiversity

INTRODUCTION

Rice (*Oryza sativa* L.) belongs to the family Gramineae. It is one of the major food crops of the world and forms the staple diet for about half of the world's population. Asia is the leader in rice production contributing to about 90% of the world's produce. Over 75% of the world rice produce is consumed by people in Asian countries which makes it an important component for the food security of Asia. Rice has been considered as the queen among cereals for its nutritional quality and higher digestibility and it has played a pivotal role in shaping the cultures, diets, and economies of billions of people. The state of Odisha is known for its unique rice land races. The first collection of 1,745 types of rice landraces was done from a small tract in Jeypore (under undivided Koraput district) representing practically the entire range of genetic variability and it helped in establishing the region as the "Secondary centre of origin of cultivated rice" (Ramiah and Ghosh, 1951; Govindswamy and Krishnamurty, 1958). The tribal farmers adopt age-old cultivation practices and grow a number of traditional rice varieties timed to mature in months matching festive or ritual occasions. The traditional life style of these people has always been insulated from the present modern ways of life and comforts. The rice landraces found in Odisha represent a wide range of genetic variability particularly for more useful characteristics such as growth in various land types (upland, medium land, lowlands etc.), possession of strong aroma, drought tolerance nature, stable yield (without use of chemical fertilizers), weed competitiveness, moderate tolerance to pests/diseases, good eating and cooking quality, higher grain number, suitability for various fast-food preparations etc.

There are three main developmental stages in rice: germination/ vegetative growth, reproductive development and grain ripening and seed germination is an early and crucial stage in the life cycle of rice plants and refers to the physiological processes starting from the uptake of water by the dry seed and ending with the radicle protrusion (Bewley, 1997). It is a complex physiological and biochemical process that involves a series of signal transduction and gene expression regulation. Rice seed germination could determine its seedling growth and yield to some extent. A series of exogenous and endogenous factors contribute in germination regulation, including water, temperature, light, circadian rhythm, and phytohormones (Penfield etal., 2005; Holdsworth et al., 2008). Germination and seedling growth are very important for the early establishment of plants and this in turn directly affects the gross photosynthetic and respiration rates as well as the activity of ATPase.

REVIEW OF LITERATURE

The seed is a miniature plant in a latent state, encompassing all the characteristics of the cultivar to which it belongs. It is the terminal point in the life cycle of the mother plant as well as the starting point in the life cycle of the plant that follows it. The transition of the seed from the resting phase to one of activity is known as germination (Gelmond, 1981). Evenari 1961 defined germination as "the sum total of all the physiological processes occurring inside the seed, which starts with imbibition of water and ends with protrusion of the embryonic root in docots and coleororhiza in monocots." Ching, 1972 defined germination as a stage in the "developmental process from fertilized egg cell to mature plant which is genetically programmed and environmentally modulated." Each developmental phase exhibits a characteristic pattern of metabolism controlled by enzyme activities that differ in kind, rate and location. The rate of enzyme activities are controlled by the quantity of the active enzyme, substrates(s), cofactor(s), coenzyme(s), presence of inhibitors or stimulators, physical and chemical micro-environment including temperature, light, pH, hydration, ionic strength etc.

Seed is the most important part of a plant for continuity of life and race and its protection and preservation is also equally important. Germination is the first important event of plant life. The second important event of plant life after germination is seedling growth in which the new areas of the tiny plant develop and the third important event being seedling establishment where the seedling interacts with the environmental factors and survive. During this process of seedling growth, all necessary constituents of the cell, cell-wall and cell inclusions are synthesized which

are utilized for growth, development and stabilization of the seedlings. These events are also directly or indirectly influenced by various environmental and internal factors. During this stage, the seedlings try to become self-established by developing root and shoot systems. The growth of both root and shoot systems are also controlled by various metabolic activities carried out by leaves. Hence, changes in shoot and root length of the seedlings, their fresh and dry weights, changes in certain macromolecular contents such as chlorophylls, other pigments, biomolecules etc. are considered as important parameters of seedling establishment.

High percentage of seed germination and seedling establishment, disease free seedling and healthy growth of the plant are considered to be some of the noteworthy indications about high yield potential of any crop plant. In nature, as the plants are very much exposed to different environmental changes, insects, pests, they suffer from various types of diseases at different stages of their life cycle. So, the plants cannot maintain a perfect disease free life, unless proper care is being taken. The seeds produced from the disease affected plants cannot be utilized in agriculture or for food purposes because these lack germinating vigour and nutritional value.Though the rice plants are very much susceptible to various types of diseases and the production decreases significantly which is strongly related to the degree of infection still it is considered to be the staple food of almost half of the world's population. In India, more than 37,793,000 hectors of land is under rice cultivation and 75% of Indian population depends upon rice as staple food. The cultivation of this cereal crop is a challenging task for a cultivator because it needs a lot of experience and much care. All phases of its life cycle : i) germination phase, ii) seedling phase, iii) growth and tillering phase, iv) flowering phase, v) fruiting phase and vi) harvesting phase are very much sensitive to pest infection and also to changes in the climatic conditions (Chatterjee and Maiti, 1981). Out of all the phases, the germinating phase needs more attention because it is the basic and most sensitive phase from which the life cycle of the plant starts.

MATERIALS AND METHODOLOGY

Sample Collection

Grains of 10 rice landraces were collected from the tribal farmers of Rayagada, Koraput, Malkangiri, Phulbani districts of the southern part of Odisha during the months of July- August. Sample grains of each variety were stored in self-sealing plastic bags at ambient temperature under moisture free conditions in the laboratory for further studies.

Equipments, Chemicals, Labware and tools

All the chemicals used were of analytical grade and procured from Himedia Pvt Ltd. India, Sigma Aldrich India, Merck Pvt Ltd., India. The glasswares and plastic wares were procured from Borosil Glass Works Ltd., India and Tarsons Products Pvt Ltd. respectively.

Equipments and tools used

Digital Balance (Shimadzu BL220H), Dhona balance, pH meter (Eutech pH tutor), Hot air oven, Incubator (C1-3S), refrigerated centrifuge (Remi C-24B), benchtop centrifuge, vortexer, waterbath shaker (Remi), burril shaker, UV double beam Spectrophotometer (Shimadzu 01482), laminar air flow cabinet, micropipettes (0.5-10µls, 5-50 µls & 200-1000 µls), germinator, Photo-Warburg's apparatus (New Paul, India), Whatman No. 42 filter paper.

Studies relating to germination

Studies on seed germination were performed by sowing the grains of each variety in earthen pots during the month of July. Soil having pH of 8.6 and an ambient temperature of 28-30°C was selected for seed sowing .The success rate of germination was calculated for each of the rice landraces under study after 10 days of sowing. The following tasks were performed following the germination of seeds:

Seedling height

Seedling height was measured at the 5 leaf stage. Height is recorded in cm from the base of the shoot to the tip of the tallest leaf blade (IBPGR-IRRI Rice Advisory Committee, 1980).

Study of seed viability

The seeds were soaked with different concentrations of test solution from 12h to 96h. After scheduled period of exposure, the seeds were washed with tap water, followed by distilled water and the seed viability was tested according to the procedure of (Moore 1969). The result was expressed as percentage of mortality.

Experimental methods of seed treatment

Always 25 no. of grains and 50ml seed dressing solution were utilized for single treatment. Usually the seeds were kept inside the nylon netted cloth and then allowed to dip inside the test solution for desired period of time. After treatment the seeds were taken out and then these were further allowed to dry on a blotting paper at room temperature and in shade condition. During treatment the seed dressing solution was under constant shaking by magnetic stirrer. After treatment the test solution was rejected. The above procedure was repeated according to the need of the number of replicates for a particular type of experiment. The seeds were arranged on the petriplates and enough care was taken to see that the seeds remain in contact with the medium and the seeds do not dip-in the medium. The petriplates were kept in the culture racks and also in the seed germinator (Remi). The medium was never allowed to be dried. The exact amount of water required was supplied in equal quantity to maintain constancy.

Always twenty five seeds were kept in each petriplates and each treatment including control. For germination and growth studies mainly out of two types of treatments, short term treatment was conducted in petriplates both in racks and seed germinator. Thereafter the set was regularly supplied with distilled water at an interval of 12 hours. In all sets, the seeds were allowed to germinate in normal photo inductive cycles (PIC), normal humid atmosphere and at a temperature of $26 + 2^0$ C for 48 hours. After 48 hours of normal soaking and incubation, all seedlings were transferred to growth chambers, culture rack and seed germinator [Remi]. To calculate the percentage of seed germination, periodical observations were made at an interval of 24 hours to 144 hours. First emergence of coleorhizae (Referred as Root) about 2 mm in length was considered as normal germination, so also appearance of coleoptiles (referred to as shoot) before emergence of coleorhizae was considered as abnormal germination. From this pilot test, a range was selected by visual screening and percentage of germination and percentage of seedling establishment was noted. The seeds were allowed to grow in petriplates inside the growth chamber. Visual screening was carried out basing on the growth and the percentage of seed germination and percentage of seedling establishment was also calculated. Care was taken to avoid contamination during the experiments.

Study of seedling growth (Petriplate Culture)

In petriplate culture, the petriplates were cleaned with tap water then with chromic acid and then tap water and finally with double distilled water and dried in an oven. Twenty five pre soaked seeds were sown in petriplates at uniform distance in all the sets. All the petriplates were kept at room temperature and normal photo-inductive cycle was maintained by providing light from fluorescent tubes in day time. On each 7^{th} day of exposure, seedlings were harvested for respective experimental analysis.

Study of Morphological Parameters

Shoot length and Root length

From each replicate 10 seedlings were selected randomly and shoot and root lengths were measured, with the help of a scale.

Shoot Weight and Root Weight

Ten seedlings from each replicate were taken. The shoots were separated from the roots. These were washed thoroughly with distilled water, surface dried by means of blotting paper. Then fresh weights of roots and shoots were taken separately by a single pan electrical balance (Dhona). The weighed shoots and roots were kept in an oven for 48 hours at a temperature of 80^0C and their dry weights were recorded at 24h interval till we get a constant weight of the samples.

Percentage of moisture content

Percentage of moisture content was calculated as follows:

$$\text{Percentage of moisture content} = \frac{W_1 - W_2}{W_1} \times 100$$

Where, W_1 = Fresh weight; W_2 = Dry weight

Photosynthetic efficiency

Pigment studies

To study the pigments (total chlorophyll, total phaeophytin and carotenoid content) the pigment was extracted in 10 ml of cold 80% acetone with a pre-chilled micro-tissue homogenizer of the shoot tissue, centrifuged at 8000rpm for 10 minutes and the supernatant was taken and the extinction values at 475, 649 and 665nm were recorded to estimate total carotenoid and total chlorophyll, respectively. From the above supernatant, 5 ml was pipetted into a stoppered test tube, a pinch of oxalic acid was added, shaken thoroughly and was kept in a refrigerator overnight for estimation of phaeophytin. The total phaeophytin was measured by recording the extinction values of the extract at 655 and 666 nm. The amount of total chlorophyll and total phaeophytin was calculated by using the formula given by Vernon (1960). The amount of carotenoid was calculated by using the formula given by Davies (1976).

Total chlorophyll (mg l^{-1}) = (6.45 x OD at 665 nm) + (17.22 x OD at 649 nm)

Total phaeophytin (mg l^{-1}) = (6.75 x OD at 666 nm) + (26.03 x OD at 655 nm)

$$\text{Carotenoid content (mg } l^{-1}) = \frac{D\ V\ K}{2500 \times 100}$$

Where, D = Optical density at 475 nm;

V = Volume of the extract,

K = Dilution factor;

2500 = Specific extinction coefficient at 475 nm

Oxygen evolution and consumption measurements

The evolution of oxygen due to photosynthesis and consumption of O_2 in respiration were measured manometrically with the help of a Photo-Warburg's apparatus (New Paul, India) following the procedure of Hannan and Patouillet, 1972 and Oser, 1965. Rate of photosynthesis was expressed in µl of O_2 evolved hr^{-1} g^{-1} of the seedling and respiration rate was expressed in µl of O_2 consumed hr^{-1} g^{-1} of leaves of the seedling. The GPP (Gross Primary Production) and NPP (Net Primary Production) values were calculated from the values obtained from both the oxygen evolution and oxygen consumption studies. The above studies were conducted for 144hr old seedlings in petriplate culture.

The freshly weighed plant tissue was suspended inside the Warburg's flask with 0.25 ml of sucrose solution (0.25 M) and base medium. The central well of the Warburg's flask contain a wick Whatman filter paper soaked in 10% KOH solution to absorb carbon dioxide produced during the experiment. Triplicate manometers were used simultaneously

with adequate thermo-barometers for necessary corrections. The flasks were acclimatized with the temperature and light intensity for 15 minutes with normal shaking (74-78 strokes / minute) of the apparatus. Then the oxygen evolution was recorded after air tightening the Warburg's flask with normal shaking. The filter paper wick was removed and the entire KOH was soaked. The flask was air-tightened and the Warburg flask was again acclimatized for 15 mins after light was flooded (2200+200Lux).The evolution of oxygen was therefore recoded by the change indicated in the closed arm of the manometer. The readings were multiplied by flask constant and other factors (Sahu, 1987) (a factor, determined earlier for each Warburg flask). Rate of photosynthesis was expressed in µl of CO_2 consumed/ sample (rice seedlings) / hr and respiration rate was expressed in µl of CO_2 produced / sample of seedling / hr.

ATPase activity, extraction and assay

The plant material was grounded with 10 ml of 0.1 M Tris-HCl buffer (pH 7.4) in pre-chilled micro-tissue homogenizer and the crude homogenate was centrifuged at 4°C and 10,000 rpm for 20 minutes. The supernatant was used as the sources of enzyme. The assay mixture consisted 2 ml of 0.1 M Tris-HCl buffer (pH- 7.4), 1 ml of $MgCl_2$ (20 m mol), 1 ml of ATP solution in buffer (1 m mol/ ml) and 1 ml of enzyme extract. The assay mixture was incubated at 37°C for 30 minutes and the reaction was stopped by adding 1 ml of 20% perchloric acid. A zero time control was run at the same time with the enzyme extract added after perchloric acid to the assay mixture. The assay mixture were then kept in a refrigerator for 30 minutes and centrifuged. An aliquot of the supernatant was taken for estimation of inorganic phosphate by Molybdenum blue method (Martineck, 1970). Colour development proceeds at room temperature for 30 minutes and the extinction was measured at 600 nm by a digital spectrophotometer (UV-Visible Spectrophotometer, PC based, Systronics, 119). The amount of inorganic phosphate was calculated from a standard graph prepared by a graded series of known concentrations of Potassium dihydrogen phosphate (KH_2PO_4). Activity of ATPase was expressed as mg of inorganic phosphate (Pi) liberated / hr /100 mg dry weight of the leaf tissue. All the experiments were performed in triplicates and repeated thrice. The observed results were statistically analysed to test the level of significance and validity of the data.

The germination success rate of the selected varieties varied between 81.8- 100%. Varieties Kanakchudi, Muktabali, Kalamalli, Kandulakathi, Dudhamani and Sapuri showed 100% germination whereas 81.8% germination was found withS the varieties Asamchudi, Baunsidubraj and Deulabhoga. The variety Tikichudi showed 90.9% success rate. All the selected varieties showed dwarf habit. The height increase per day was also calculated for each of the selected varieties and the values ranged between 0.93- 2.11. Table 1 and Fig 4 Showed the changes in percentage of seed germination and seedling establishment, root and shoot length and lateral roots in 10 varieties of rice seedlings after 144hrs of exposure. Out of 10 varieties tested varieties V2-Asamchudi and V5- Kanakchudi showed 100% germination and 100% seedling establishment when compared to rest 8 varieties of rice. Tikichudi, Kalamalli and Sapuri showed 80% germination and 80% seedling establishment was recorded in Kalamalli but in case of Tikichudi and Sapuri, 70% seedling establishment was recorded (Fig.12). Deulabhoga seeds showed 45% germination and 30% seedling establishment which is not statistically significant. Baunsidubraj, Muktabali and Dudhamani showed 35%, 28%, 15% germination and 12%, 11%, 07% seedling establishment, respectively. These values are far less significant (Fig. 4 and Table 2).

Table 2 showed very interesting results pertaining to lateral roots. In case of Deulabhoga, the root length was 9.2cms whereas in the rest of the varieties, the root length was less when compared to Deulabhoga. The least number of lateral roots were found in Dudhamani, Muktabali and Deulabhoga. In case of Kanakchudi and Tikichudi maximum number of lateral roots were observed as it is good sign for this monocot plant (Table-22 and Fig. 13). Longest shoot length was recorded in case of Asamchudi, Deulabhoga and Kanakchudi and least shoot length was recorded in case of Dudhamani. The rest of the varieties showed stunted growth. It seems varieties like Tikichudi, Baunsidubaraj, Muktabali, Kalamalli, Kandulakathi and Sapuri showed growth but not like the same as these varieties showed at

Koraput district. It seems these varieties are not responding well to laboratory controlled conditions. It seems the climatic conditions of Koraput district play a crucial role due to which all these varieties respond well to Koraput climate rather than Ganjam or Bhanjabihar climate. The least number of lateral roots in Dudhamani, Muktaballi and Deulabhoga indicated the least growth and production both vegetative and reproductive indicating least grain production. These three varieties are considered to be the least productive among the 10 varieties tested which warrants attention (Table 2). From root and shoot length measurements, it can be inferred that the varieties like Asamchudi, Tikichudi, Kalamalli, Sapuri, Deulabhoga and Kandulakathi may be considered as the best for cultivation when compared to the rest of the varieties (Fig 5 and Table 2).

Table 2 and Figures 6 and 7 showed the changes in root and shoot fresh weight and dry weight of 10 varieties of rice seedlings after 144hrs of exposure. Varieties such as Deulabhoga, Muktabali and Dudhamani showed the lowest fresh and dry weight in roots and shoots of 144hr old seedlings. Asamchudi, Kanakchudi and Kandulakath showed the highest biomasss when compared to rest of the varieties. The variation in weight was probably due to the high photosynthetic potential of the varieties and may be these varieties showed best adoptive features to the present environmental conditions available in the laboratory. Table-2 indicated the moisture content of the 144hr old seedlings. The observations were mostly as expected. Baunsidubraj, Muktabali and Dudhamani showed the lowest moisture content in the seedlings. Moisture content of the seedlings plays a crucial role for the plant growth and development. The survival of the seedlings depends mostly on the moisture content of the seedlings and all metabolic processes are directly related to the water content available in the seedlings (Fig. 16). In low water level, a shunted growth is expected. The depletion in metabolic activity can be linked to moisture content and also in seed biological studies moisture plays an important role during germination.

As sufficient water was available in the experimental plates, deficit of water is not the limiting factor. It may be because of low imbibition rates of the seeds which affected the mobilization of biochemicals at the time of germination and seedling growth that lead to decrease in growth and shunted growth of the seedlings. The differential behaviour of the seeds can also be correlated to storing conditions, use of seed dressing chemicals, age of the seeds. Some of the seeds might have lost their viability and vigour during holding time. However, few seeds germinating in a particular condition and other seeds do not germinate in those conditions probably indicate the mixture of seeds belonging to different viability groups.

Figure 7 related to dry weight analysis followed the same trend like that of figure 6 related to fresh weight of the seedlings as expected. Fig.16 indicated the changes in moisture content in root and shoot of 144hr old seedlings of 10 different varieties of rice seeds / grains conducted under laboratory controlled conditions. The following varieties showed the highest moisture content: Sapuri-84.8%, Kanakchudi- 83.6%, Kandulakathi- 83.3%, Asamchudi-82.8% and the rest of the varieties showed significantly less moisture content in the 144hr old seedlings. Baunsidubraj, Muktabali and Dudhamani showed the lowest moisture content when compared to the rest of the varieties. This low water content probably harmed the survivability of the seedlings. As described earlier the moisture content plays a key role in early phases of germination of the seeds and the seedling growth depends upon the moisture content.Table 4 and figure 9 Showed the changes in gross photosynthetic rate in 144hr old seedlings in 10 varieties of rice seedlings after 144hrs of exposure. Asamchudi showed 248.4±15.6µl of O_2 evolved g.-1 hr.-1, Kanakchudi showed 239.7±14.1µl of O_2 evolved g.-1 hr.-1, Tikichudi showed 231.9±11.5µl of O_2 evolved g.-1 hr.-1 and Deulabhoga showed 221.5±17.3µl of O_2 evolved g.-1 hr.-1 gross primary production or photosynthetic rate in 144hr old seedlings. In rest of the varieties the photosynthetic rate was significantly less. The least photosynthetic rate was marked in case of Dudhamani variety 157.6±11.3µl of O_2 evolved g.-1 hr-1. Significantly low values of photosynthetic rate were also observed in Muktabali and Baunsidubraj where the values were 169.4±16.3µl of O_2 evolved g.-1 hr-1and 162.7±11.8µl of O_2 evolved $g^{-1} hr^{-1}$ (figure 9 and table 4).

Table 4 and figure 9 Showed the changes in respiration rate in 144hr old seedlings in 10 varieties of rice seedlings after 144hrs of exposure. Asamchudi showed 236.6±11.4µl of CO_2 evolved g^{-1} hr^{-1}, Kanakchudi variety showed 214.5±13.2µl of CO_2 evolved g.-1 hr.-1, Tikichudi variety showed 228.7±9.8µl of CO_2 evolved g.-1 hr.-1 and Deulabhoga showed 201.5±12.4µl of CO_2 evolved g^{-1} hr^{-1} respiration rate in 144hr old seedlings. In rest of the varieties, the respiration rate was significantly less. The least respiration rate was marked in case of Baunsidubraj variety 148.3±6.5µl of CO_2 evolved g^{-1} hr^{-1}. Significantly low values of respiration rate was observed in Muktabali and Dudhamani where the values were 165.8±19.4µl of CO_2 evolved g^{-1} $hr^{-1}$and 151.3±9.3µl of CO_2 evolved g^{-1} hr^{-1} respectively (Fig. 9 and Table 4).

Table 4 and figure 10 showed the changes in ATPase activity in 144hr old seedlings in 10 varieties of rice seedlings after 144hrs of exposure. Kanakchudi showed 4.24±0.37µg of ip liberated/ hr/ 100mg dry wt., Asamchudi showed 4.14±0.43µg of ip liberated/ hr/ 100mg dry wt., Sapuri showed 4.09±0.61µg of ip liberated/ hr/ 100mg dry wt., Tikichudi variety showed 3.82±0.54µg of ip liberated / hr / 100mg dry weight and Deulabhoga showed 3.5±0.56µg of ip liberated / hr / 100mg dry weight ATPase activity in 144hr old seedlings in the descending order. In rest of the varieties the ATPase activity was significantly less. The least ATPase activity was observed in case of Dudhamani which was 2.25±0.24µg of ip liberated/ hr/ 100mg dry weight. Significantly low values of ATPase activity was observed in Muktabali and Baunsidubraj where the values were 2.47±0.53µg of ip liberated/ hr/ 100mg dry wt. and 2.63±0.61µg of ip liberated / hr / 100mg dry wt. (Fig. 10 and Table 4).

Table 5 and Fig. 11 showed the changes in chlorophyll content in 144hr old seedlings in 10 varieties of rice seedlings after 144hrs of exposure. Kanakchudi showed 1.996 mg of chlorophyll/ liter, Asamchudi showed 1.992 mg of chlorophyll/ liter, Sapuri showed 1.935 mg of chlorophyll/ liter, Tikichudi showed 1.981 mg of chlorophyll / liter, Kalamalli showed 1.974 mg of chlorophyll / liter, Kandulakathi 1.965 mg of chlorophyll / liter and Deulabhoga showed 1.714 mg of chlorophyll / liter in 144hr old seedlings in the descending order. In rest of the varieties the chlorophyll content was significantly less. The least chlorophyll content was marked in case of Dudhamani which was 1.588 mg of chlorophyll/ liter. Significantly lower values of chlorophyll content was observed in Muktabali and Baunsidubraj in which 1.622 mg of chlorophyll/ liter and 1.658 mg of chlorophyll/ liter was found respectively (Fig. 11 and Table 5).

Table 5 and Fig.11 showed the changes in phaeophytin content in 144hr old seedlings in 10 varieties after 144hrs of exposure. Asamchudi showed 1.346 mg of phaeophytin/ litre , Kanakchudi showed 1.342 mg of phaeophytin/ litre, Sapuri showed 1.302 mg of phaeophytin /litre, Tikichudi showed 1.311 mg of phaeophytin /litre , Kalamalli showed 1.322 mg of phaeophytin /litre, Kandulakathi 1.105 mg of phaeophytin / liter and Deulabhoga showed 1.101 mg of phaeophytin / liter in 144hr old seedlings in the descending order. In rest of the varieties the phaeophytin content was significantly less. The least phaeophytin content was found in case of Dudhamani which was 1.009 mg of phaeophytin / liter. Significantly low values phaeophytin content was marked in Muktabali and Baunsidubraj where the values were 1.114 mg of phaeophytin/ liter and 1.066 mg of phaeophytin/ liter respectively (Fig. 13 and Table 5). Table 5 and Fig.13 showed the changes in carotenoid content in 144hr old seedlings in 10 varieties of rice seedlings after 144hrs of exposure. Kanakchudi showed 0.000386mg of carotene/ liter, Asamchudi showed 0.000384mg of caroterne / liter, Tikichudi showed 0.000381 mg of carotene/ liter, Kalamalli showed 0.000378mg of carotene/ liter, Sapuri showed 0.000376mg of carotene / liter, Kandulakathi 0.000269 mg of carotene / liter and Muktabali showed 0.000274 mg of carotene / liter in 144hr old seedlings in the descending order. In rest of the varieties the carotene content was significantly less. The least carotene content was marked in case of Dudhamani which was 0.000198 mg of carotene/ liter. Significantly lower values of carotene were found in Deulabhoga and Baunsidubraj which were 0.000262 mg of carotene/ liter and 0.000245 mg of carotene/ liter respectively (Fig.12 sand Table 5).

The differences in chlorophyll content is linked to photosynthesis and gross production and a higher chlorophyll level will indicate higher production and lower chlorophyll level indicates stress. Padhy (2006) clearly opined that different climatic factors have major impact on the chlorophyll content, rate of photosynthesis and production.

CONCLUSION

Out of the ten varieties tested for the seed biological studies, it was evident that the six varieties like Kanakchudi, Asamchudi, Tikichudi, Kalamalli, Sapuri and Kandulakathi were the best varieties which can be cultivated in all agroclimatic conditions. Dudhamani variety can only be grown in Koraput district and this variety will not suit to all agroclimatic conditions. The present study at base level in seed biology will only indicate the status of the system under study. Detailed biochemical and enzymatic analysis of all the available varieties can give us some interesting information regarding the variation in the biological characteristics of the varieties. In addition, molecular profiling and sequencing data using the tools of biotechnology can hint at the phylogenetic relationships among the studied rice landraces. Further the biochemical and nutritional evaluation of the studied races would pave ways for the successful exploitation of these rice landraces in food fortification processes to combat elemental and nutritional deficiencies and the results of the study would also provide a means for the conservation of these neglected races.

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Fig 1. Rice landraces used for the study (as known by their local names)

Fig 2. showing germination of the rice seeds after 10 days of sowing.

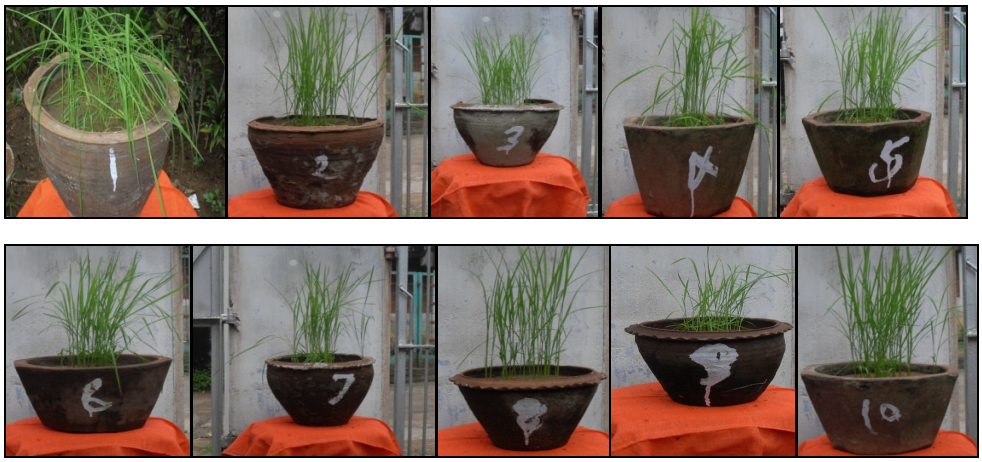


Fig 3. showing growth after 30-days of germination of the studied rice landraces

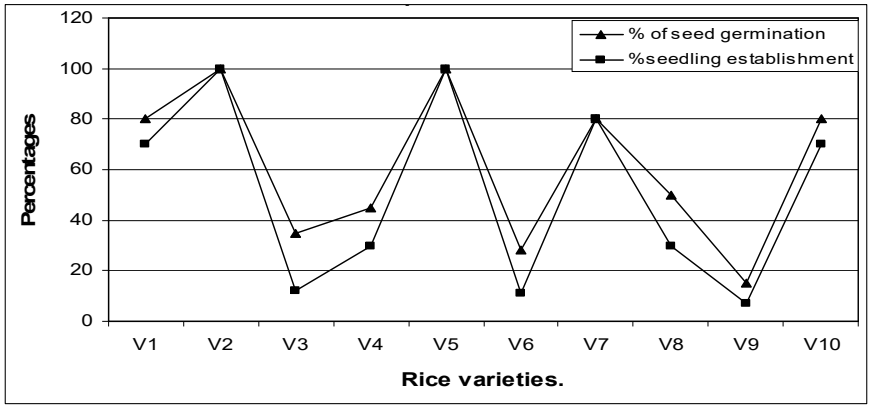


Fig 4.Changes in % of seed germination and seedling establishment of 10 varieties of rice grains after 144 hrs of exposure.

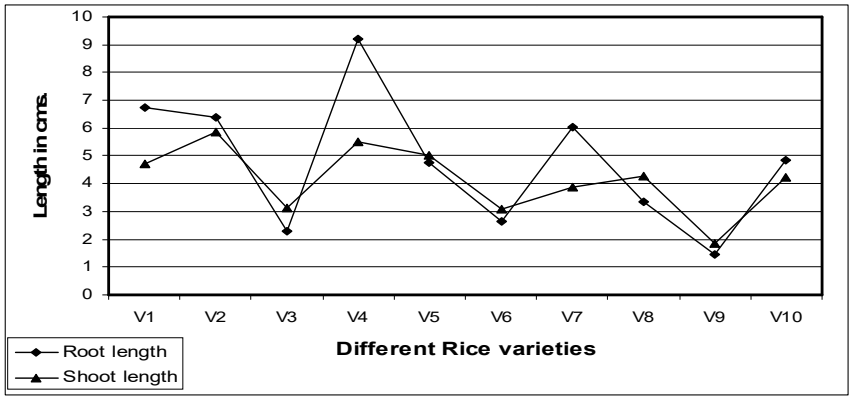


Fig 5. Changes in root and shoot length in 10 different varieties of rice after 144 hrs of germination

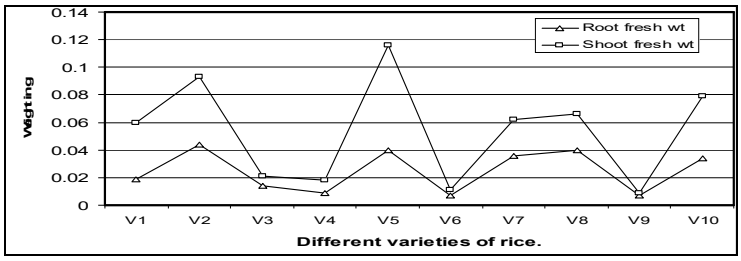


Fig 6. Changes in root and shoot fresh weight of seedlings after 144 hrs of germination in different varieties of rice landraces.

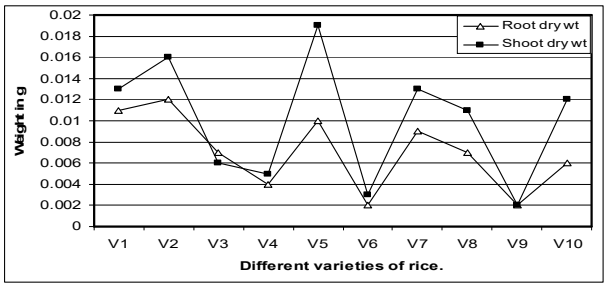


Fig 7. changes in shoot and root dry weight of 144 hr. old seedlings in different varieties of rice.

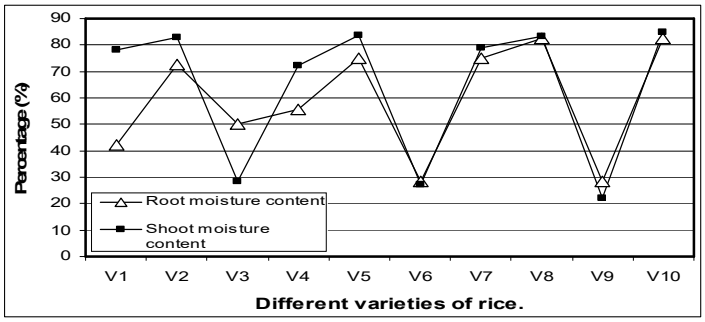


Fig 8. showing changes in moisture content in root and shoot of 144 hrs old seedlings of different varieties of rice

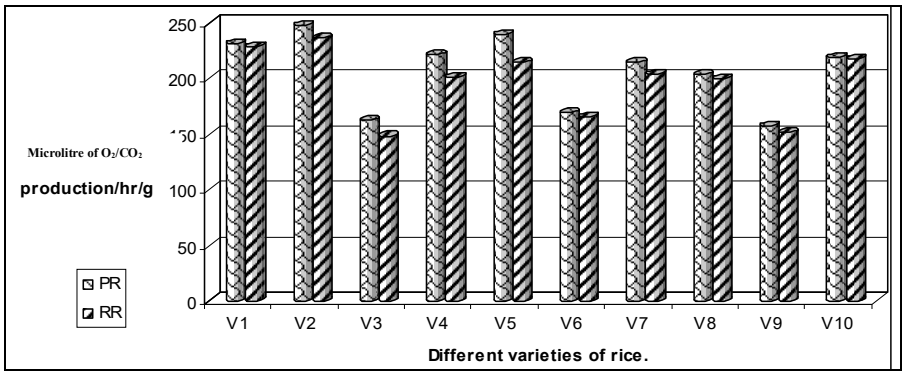


Fig 9. Changes in gross photosynthetic rate and respiration rate in 144 hr. old different varieties of rice seedlings grown in laboratory controlled conditions.

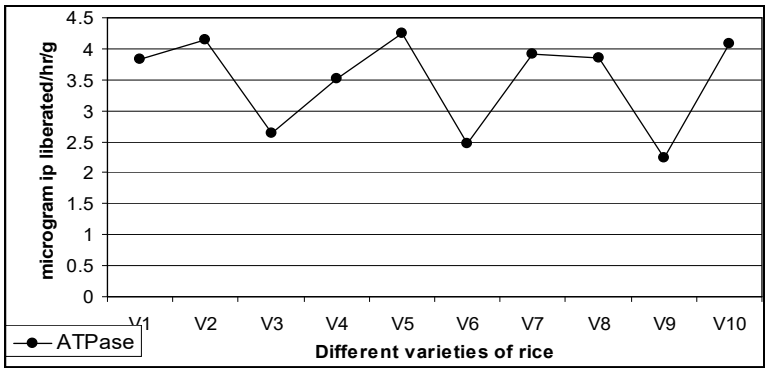


Fig 10. Changes in ATPase activity in 10 different varieties of 144 hr. old seedlings.

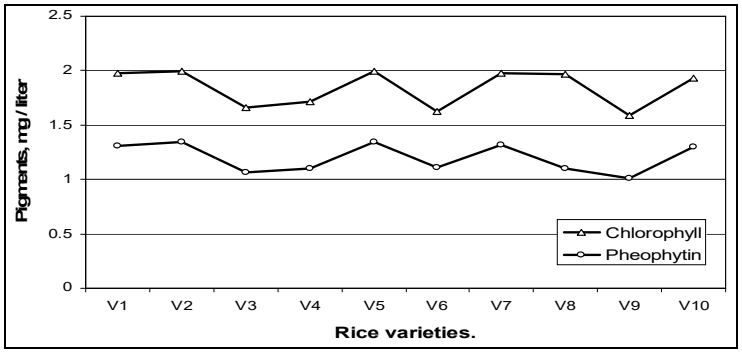
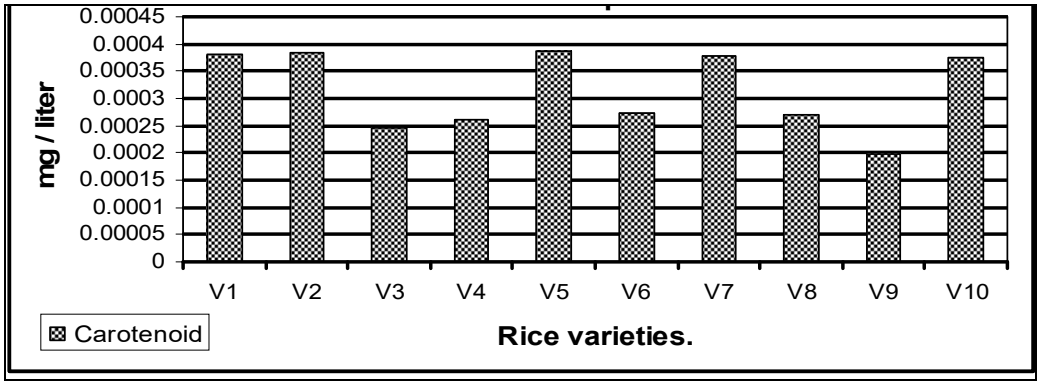


Fig 11. Changes in chlorophyll and pheophytin content in the leaves of 144 hr. old seedlings in 10 varieites of rice



*Data are the mean of the samples

Fig 12. Changes in carotenoid content in the leaves of 144 hr old seedlings in 10 varieities of rice.

Table 1. Germination success rate and plant characteristics of rice landraces

Variety	% Success	Height of Plant in 30 days (cm)	Height increase per day (cm)	Habit
Jp1	90.9	58.20	1.94	Dwarf
Jp2	81.8	51.36	1.71	Dwarf
Jp3	81.8	63.36	2.11	Dwarf
Jp4	81.8	47.76	1.59	Dwarf

Jp5	100	56.86	1.89	Dwarf
Jp6	100	58.63	1.95	Dwarf
Jp7	100	61.19	2.03	Dwarf
Jp8	100	53.65	1.78	Dwarf
Jp9	100	28.18	0.93	Dwarf
Jp10	100	44.45	1.48	Dwarf

Table 2 Showing the changes in percentage of seed germination and seedling establishment, root and shoot length and lateral roots in 10 varieties of rice seedlings after 144hrs of exposure. (Data are the mean of three replicates).

Sl. No.	Name of the rice variety	Percentage of seed germination	Percentage of seedling establishment	Root length in cm	Shoot length in cm	No. of lateral roots
V1	Tikichudi	80	70	6.72	4.7	10.6
V2	Asamchudi	100	100	6.38	5.88	7.6
V3	Baunsidubraj	35	12	2.28	3.12	4.5
V4	Deulabhoga	45	30	9.2	5.5	2.2
V5	Kanakchudi	100	100	4.74	5.04	10.0
V6	Muktabali	28	11	2.65	3.08	1.4
V7	Kalamalli	80	80	6.02	3.88	8.0
V8	Kandulakathi	50	30	3.35	4.275	5.5
V9	Dudhamani	15	07	1.45	1.84	1.2
V10	Sapuri	80	70	4.86	4.22	6.2

Table 3. Showing the changes in root and shoot fresh and dry weight and moisture content in 10 varieties of rice seedlings after 144hrs of exposure (Data are the mean of samples).

S.No.	Name of the rice variety	Root fresh weight(g)	Root dry weight(g)	Shoot fresh weight(g)	Shoot dry weight(g)	Root moisture content (%)	Shoot moisture content (%)
V1	Tikichudi	0.019	0.011	0.060	0.013	42.10	78.33
V2	Asamchudi	0.044	0.012	0.093	0.016	72.72	82.79
V3	Baunsidubraj	0.014	0.007	0.021	0.006	50.00	28.57
V4	Deulabhoga	0.009	0.004	0.018	0.005	55.55	72.22
V5	Kanakchudi	0.040	0.010	0.116	0.019	75.00	83.62
V6	Muktabali	0.007	0.002	0.011	0.003	28.57	27.27
V7	Kalamalli	0.036	0.009	0.062	0.013	75.00	79.00
V8	Kandulakathi	0.040	0.007	0.066	0.011	82.5	83.33
V9	Dudhamani	0.007	0.002	0.009	0.002	28.57	22.22
V10	Sapuri	0.034	0.006	0.079	0.012	82.35	84.81

Table 4. Changes in gross photosynthetic rate, respiration rate and ATPase activity in 10 varieties of rice seedlings after 144hrs of exposure (Data are the mean of samples ± standard deviation).

Sl. No.	Name of the rice variety	Gross Photosynthetic rate. µl of O_2 evolved $g.^{-1}$ $hr.^{-1}$	Respiration rate. µl of CO_2 evolved $g.^{-1}$ $hr.^{-1}$	ATPase activity. µg of ip liberated/hr/100mg dry wt.
V1	Tikichudi	231.9±11.5	228.7±9.8	3.82±0.54
V2	Asamchudi	248.4±15.6	236.6±11.4	4.14±0.43
V3	Baunsidubraj	162.7±11.8	148.3±6.5	2.63±0.61
V4	Deulabhoga	221.5±17.3	201.5±12.4	3.5±0.56
V5	Kanakchudi	239.7±14.1	214.5±13.2	4.24±0.37
V6	Muktabali	169.4±16.3	165.8±19.4	2.47±0.53
V7	Kalamalli	214.5±11.5	204.1±18.3	3.92±0.32
V8	Kandulakathi	203.5±7.6	199.8±24.5	3.86±0.47
V9	Dudhamani	157.6±11.3	151.3±9.3	2.25±0.24
V10	Sapuri	219.4±11.4	218.2±9.8	4.09±0.61

Table 5. Showing the changes in pigment content in 10 varieties of rice seedlings after 144hrs of exposure (Data are the mean of samples).

Sl. No.	Name of the rice variety	Chlorophyll content, mg / liter	Phaeophytin content, mg / liter	Carotene content, mg / liter
V1	Tikichudi	1.981	1.311	0.000381
V2	Asamchudi	1.992	1.346	0.000384
V3	Baunsidubraj	1.658	1.066	0.000245
V4	Deulabhoga	1.714	1.101	0.000262
V5	Kanakchudi	1.996	1.342	0.000386
V6	Muktabali	1.622	1.114	0.000274
V7	Kalamalli	1.974	1.322	0.000378
V8	Kandulakathi	1.965	1.105	0.000269
V9	Dudhamani	1.588	1.009	0.000198
V10	Sapuri	1.935	1.302	0.000376

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RESEARCH ARTICLE

A Statistical Approach on the Impact of COVID-19 in Procurement Management System in Construction Projects

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ABSTRACT

Procurement management plays a pivotal role in the successful execution of the project in the construction industry. On the other hand, procurement management has continued to pose significant obstacles to the building projects' progress and profitability due to Covid-19. Studies have shown that materials account for 60 percent of the total cost of the project, which clearly specifies that if any delays or mishandling occur during the procurement process; the project schedule will be affected, thus increasing the cost and time. This study attempts to identify the distinct phases of procurement management and to analyze Covid-19 attributable empirical study on the impact of the Procurement Management Process in construction projects. The project recommends key procurement areas including certain quantity of materials, designed to set standards and specifications for the materials to be procured, preparing the scope of the procurement work by the influence of Covid-19, drafting up a report on the suppliers to enhance their effectiveness, giving adequate technical and financial coordination with the suppliers to overcome the financial crisis.

Keywords: Covid-19, Empirical study, Procurement Management

INTRODUCTION

Construction projects are extremely complex and often take place in an uncontrolled, unprepared, and dynamic environment where each project is completed through several phases. Modern construction management therefore requires real-time and accurate information to be shared between all parties involved in order to carry out efficient and effective planning, as well as execution, Equipment, equipment, manpower, and resources needed to construct and execute a project. Building material contributes around 60 per cent of the overall construction value. That demonstrates how important procurement is to manage the project. Materials management is an essential function

which enhances productivity in construction projects. There is hardly any place in today's globalized world that has been left untouched by the magnitude of the Novel Corona virus or the Covid-19 pandemic. At the hands of the cruel Covid-19 almost every commercial operation is suffering. Due to the intrinsic nature of business practice, some industries may inadvertently prosper under the pandemic, while others may weather the storm. The construction and engineering sector is definitely at the wrong end of the curve, albeit with a great deal of difficulty but of the hardest affected. Efficient planning of materials procurement and storage on construction sites can lead to significant improvements in construction productivity and project profitability. Overlooking these critical interdependencies between material procurement and site-space availability can lead to serious project problems including material shortages, improper storage, poor and unsafe site layout, and productivity losses in the lockdown time. Hence, the efficient use of material has an important influence on a company's profit and can avoid delay in construction.

METHODOLOGY

The research was focused on examination of the literature, study of past documents, general interview between workers, various types of surveys and the analysis of sources of knowledge. The case study focused on building construction projects from which detailed about the procurement process of materials could be collected in the Covid-19 period. With the aid of different literature case studies and analysis of procurement management measures involved in the usual building constructions at different areas, the major problems involved in the material management processes carried out through the projects have been identified. Through this methodological approach, the different phases of this project should be clearly distinguished and the processes involved in material management have been continuously observed without failure and the root causes can be determined. The experimental analysis consists of theories and concept consideration in practice. Therefore, the present work involved in the construction site was classified as follows. Analysis of site and management, analysis of inventory controlling, analysis of purchasing procedures, analysis on procurement and tracking cost analysis. The construction and engineering sector, already facing multiple challenges, ranging from lack of capital and credit avenues to insolvencies, multiple fraud and regulatory burden under the Environmental Laws and Real Estate (Regulation and Development) Act, 2016, is now marred by the Covid-19 pandemic, with no probable relief in view. The study allowed collecting the basic data of the projects related to procurement process, approvals, purchase reports, claim reports and supply reports. From the information gathered improved strategies were obtained and a proper strategic approach to the material procurement management process was proposed for the building projects in this lockdown period.

Material Procurement

To analyze the stages in which maximum irregularities occur in the procurement process and the factors in the procurement process leading to high costs. To study the setup of the organization and factors of the site affecting the planning of the procurement in construction projects. The Objectives of material procurement are characterized by buying the best item at the right price, quantity, time and cost. The efficient as buying the best item at right Quality, Quantity, Time and Cost. The efficient material management system can bring many advantages for a company, such as reducing the overall cost of materials, improving material handling, reducing duplicate orders, materials on site when necessary and in the right quantities and improving the labor productivity, Improvements in project schedule, Quality control, Better field material control, Better relations with suppliers, Reduce of materials surplus, Reduce storage of materials on site, Labor-saving, Stock reduction, Purchase savings and Better cash flow management. This project helps to identify the gap between the procurement process and on-site use of the material at the construction stage and suggest appropriate methods and management to ensure the efficient procurement process for high quality construction projects with significantly reduced time and cost

A. Procurement Cycle

Steps to be followed in Procurement Management are:

- Requirement identification.
- Quantification of appropriate elements and preparation of requirements of procurement.
- Ensuring internal requisition and processing.
- Demanding quotes (or) for proposals.
- Assessment of propositions.
- Contract award to supplier.
- Procurement and purchasing process.
- Material delivery and inspection.
- On-site storage and handling prior to dressing.
- Return surplus stock products.

***B.* Planning**

Bill of quantities prepared by the clients in the most commonly used basis for planning things out for the project. Companies can have two main planning stages – micro and macro. The four major types of planning undertaken at sites are time, cost, material and labor. The preparation will be updated as much as possible to track whether work is processing as expected.

***C.* Purchasing**

Procedure to purchase can be described as:
Step 1 – Indent Content
Step 2 – Vendor inquiry
Step 3 –Comparison of Vendor
Step 4 – Vendor Selection and Negotiations
Step 5 – Order to purchase
Step 6 – Vendor Assessment

***D.* Ordering System**

Which materials, quantity, volume and location or distance to the site are the main problems with regard to ordering and this information will be clarified from contract documents such as the quantity bill

1. Synchronized system
2. Prescheduled ordering system
3. Periodic ordering system
4. Non-periodic ordering system

Large components such as air conditioning system, steel work, called synchronized system are ordered. The next step is large volume material like panels and a door called prescheduled ordering system; these are not as big as the synchronized system. Such materials as cement, gravel, called periodic ordering system that is required at different project stage. The small volume and large quantity are called non-periodic ordering system, such as nails and bolts.

***E.* Receiving System**

Receipt system can be divided into receipts from suppliers outside, receipts from suppliers inside. Even before the material reaches the site the receipt system starts. The three documents to be dispatched are the purchase order copy, the consulting document for suppliers and the resale note.

F. **Inspection**

Inspection can occur in two ways that is on site inspection and pre- dispatch inspection. It is the inspector's responsibility to inspect all materials delivered to the site before they are used in the work

Methods of Inspection

There are three methods of inspection:

1. Statistical
2. Visual
3. Tactile

G. **Stacking and storage**

The types of physical on-site storage system differ with the availability of space and client activities. Industrial guidelines for the loading and storage of particular materials are also considered.

Procurement management issues

A. The current faults in the Procurement management system are:

- Decision making delays and award of tender.
- Orders not done on time.
- Materials which do not match the purchase order.
- Delay in arrival of material.
- Importance of quality and the best product or service is not being realized due to lack of knowledge / improved technology.
- Excess procurement of the products and materials.
- Training shortage and ineffective management.
- Lack of communication and relationship between suppliers and contractor.

Some common problems at construction site are:

- Failure due to a timely order delaying in the project.
- Distribution which interrupts the schedule of work at the wrong time.
- False materials or mistakes in the direction of materials which require work.

B. **Delivery of Material**

Delivery of material can be divided into the following parts;

1. Issues concerning departments which consume
2. Issues for manufacturing with outside suppliers

In the case of all construction materials, on-site emitting does not occur. In case of sand or aggregate the materials are consumed according to the progress of the project as and when required. Issues are based on production program for other materials. Work order are printed based on this and the bill of materials, listing for each material. The quantity to be issued against each component requiring that material. That will control consumption automatically.

Procurement management processes

Procurement management includes the necessary processes from outside the project team to purchase or acquire products, services or outcomes needed. Project Procurement Management includes the contract management and change control processes required by authorized project team members to develop and administer contracts or purchase orders issued. Project procurement management also includes the administration of any contract issued by an external organization acquires the project from the executing organization.

a) **Procurement Plan** — This is the method of documenting a project purchase decisions, setting out the approach and identifying new sellers.

b) **Procurement Conduction** —This is the method of receiving answers from the vendor, choosing a supplier and

awarding a contract.

c) **Procurement Administer** — This is the process of overseeing, tracking contract performance, contract relationships and making adjustments and corrections where necessary

d) **Close Procurement** — This is the closure process for every procurement project.

A. Study and Analysis

The study was carried out through literature study, Questionnaire survey and virtual site case study.

B. Case Study

The case study was carried out in Major Construction Companies around Southern part of India during the Covid-19 period. Based on the detail study on case studies, factors affecting the material procurement are identified. They factors are mentioned below.

- Poor project preparation and scheduling culminated in late acquisitions.
- Delays in customer's approval of materials ended in late procurement.
- Delays in the issuance of PO (Purchase Orders) resulted in late material delivery.
- Lack of lead time to late procurement and delivery of the products.
- Poor quality of material involved in the construction site and damaged materials.
- Wrong information about the suppliers may leads to delay in the material procurement
- Current price variance causes major difference in the purchasing of materials.
- The performance of the contractual obligations is necessary or unconstitutional due to a change of circumstances beyond the control of the parties after the contract has been executed.

C. Questionnaire Survey

The Questionnaire Survey carried out with minimum fifteen members including project managers, procurement managers, contractors and consultants in each company. Data obtained from the survey were analyzed using simple percentages and Relative importance Index (RII) method

RII = ΣW÷A×N

W= the weight assigned to each strategy by the respondents A = Highest weight

N = the total number of respondents

Factors affecting Material Management are rated as

Strongly Agree (4), Agree (3), Disagree (2) and Strongly

Disagree (1).

RESULT AND CONCLUSION

Based on the on-site problems due to improper material procurement management, each problem was categorized and a cause-effect diagram was created, where factors such as consultant factors, customer, contractor, inventory, procurement, material, external factors were all addressed in general during this Covid-19 period. The various factors affecting material procurement management are listed as Contractor Contributed Factors, Owner Contributed Factors, Consultant Contributed Factors, Material Contributed Factors and External Factors. Fig 6.1 Factors affecting Material Management Nearly fifty questions were prepared and from the answers thus obtained from them were categorized into each class of problems. In this the major factors affecting the material Procurement as the first three ranks are listed below.

A)Software used for Material Management

Construction materials management software will help efficiently to produce and track purchase orders and requisitions, manage materials and back orders, and export price and cost data to multiple systems Figure. 6.2 shows 90.6% of the Organizations uses the software called BUILD SUPER FAST (BSF**)** for material management 90.6% of the organizations used MIS-MANAGEMENT INFORMATION.

B)Top Factors affecting Procurement Management

C)Cost Considered in Material Planning

The term inventory implies the cost of materials in stock at a given time. Inventory could be of raw materials, construction finishes material, tools and spares, etc**.,** there are various costs associated with Inventory Management which effects on overall process of materials management. They are purchase cost, ordering cost, carrying cost and stock out cost. A balanced inventory acts as a cushion between supply and site requirement till supplies are received. Figure. 3 shows the knowledge of considering the cost in material planning. 91% of the survey results show that most of the organizations considered all the cost involved while planning materials and only 3% of the organizations don't have knowledge about the cost involved in material planning

D)Solution

The various factors affecting the Material procurement management after the lockdown period are to be solved by the following process.

1) Late procurement of materials

a) Improper scheduling

- Wrong Material specification/quantity
- Mistakes in the schedule
- Mainly the lead time is not properly calculated

b) Lack of planning and scheduling

- Material procured without planning
- Schedule is not planned before starting the project

c) The late procurement to be avoided by the following process

- Mainly Lead time consideration for scheduling
- Plan and schedule the Materials before start the project
- Correct Material Specification and Quantity

2) Delay in approval

- Delay in approving major changes in the scope of work by Client.
- Delay in material approval by Architect
- Delay in material approval by consultants

3) Unclear and inadequate details in drawings

- Delays in updating the drawings
- Lack of details in the drawings
- Errors in the Drawings
- Drawings(Architectural, Structural, interior designs)

a) The Unclear and inadequate details in drawings to be avoided by the following process such as

- Proper coordinated drawings for services
- Advanced technology implementation
- Proper Inspection and detailed study of Drawings
- Proper update of drawing revisions
- Proper filing system of drawings
- BIM used for material applications (Clash detection, Material Specifications, revisions quantity)

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Table 1. About the Top Factors Affecting Procurement Management System

S.No	Factors affecting Procurement Management System		
	Top Factors	*RII (%)*	*Rank Order*
1.	Reducing the cost of the project materials	0.972727	**1**
2.	Quality of the materials -Past Records	0.927273	**2**
3.	Timely availability of materials	0.890909	**2**
4.	Payment Terms and Conditions.	0.881818	**3**
5.	Price competitiveness	0.863636	**4**
6.	Quality of materials.	0.845455	**4**
7.	Location of availability of material	0.845455	**5**
8.	**Wrong information about suppliers.**	**0.836364**	**5**

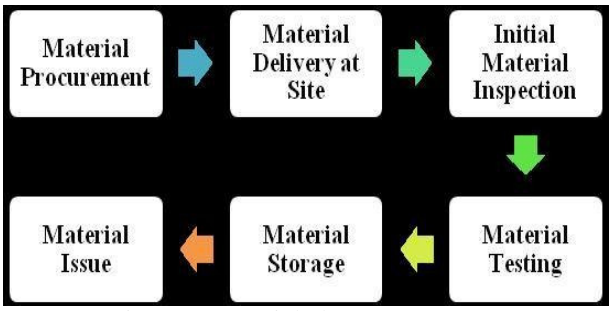

Figure 1. Material Flow Management

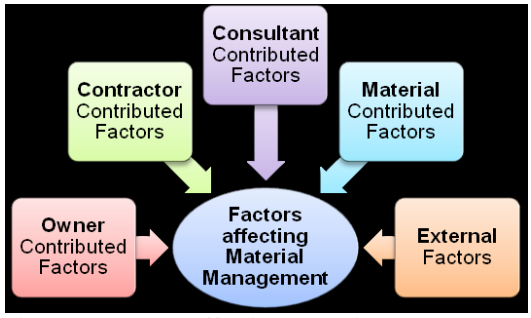

Figure 2. Factors Affecting Material Management

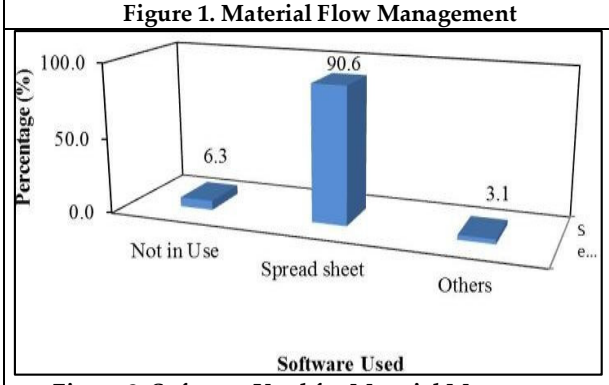

Figure 3. Software Used for Material Management

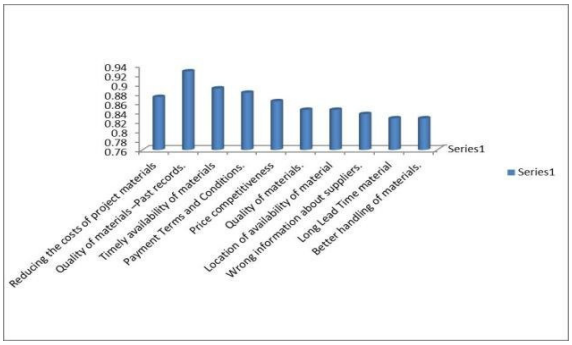

Figure 4 Top Factors Affecting Procurement

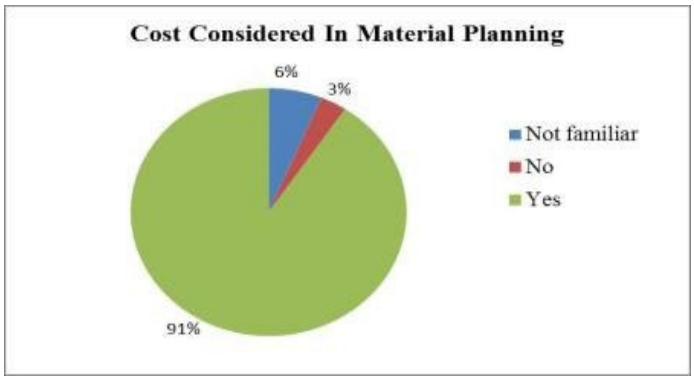

Figure 5. Cost Considered in Material Planning

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RESEARCH ARTICLE

ANN Based Speech Reorganisation System and It's Implementation

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ABSTRACT

An implementation of Artificial-Neural-Network (ANN) based speech recognition system is explored in this thesis. The fast Fourier transform (FFT) is an important operation in speech recognition, in which a great number of outing-point arithmetic operations are performed. In this thesis, we use Integer FFT to replace the Floating FFT so that the speed of speech recognition is enhanced without including the recognition rate. This uses the Hidden Markov Model (HMM) algorithm to construct speech recognition platform which causes that the speech recognition.

Keywords: ANN, HMM, FFT.

INTRODUCTION

The speech production system generates Speech signals, from our idea of understanding of signals and systems, the system characteristics depend on the design of the system. The case of the system which is linear time invariant, which is characterized in terms of its impulse response characteristics, depending on the type of input excitation the nature of response is depends to the system. For a given system to which we will use different signals like impulse response, step response, sinusoidal response etc. each of these output responses are used to understand the behaviour of the system under different conditions. In the production of speech signal the similarly phenomenon happens in which, the speech production can be broadly classified into three activities which is depending on the input excitation phenomenon. The first case where the input excitation is nearly periodic in nature, the second case where the input excitation is random noise-like in nature and third case where there is no excitation to the system. Accordingly, the speech signal can be broadly categorized into three regions. The study of these regions is the aim of this experiment.

ANN Method

The ANN is formed by connecting millions of biological neurons which are connected to each other like computer network architecture. As we biological neural network consists of dendrites, soma, nucleus, axon similarly artificial

neuron network consist of inputs, summing junction, activation function. The main objective of Artificial Neural Network is to develop a system which will perform complex task very fast then a normal traditional system with good accuracy. Each of the input and output are called nodes which are used for communication between nodes to get meaning full output.BNN can be compared with ANN as soma is as node, Dendrites are as inputs, Synapse as weights or inter connection and Axon are as outputs.

The net input is calculated by

$Y_{in}=X_1W_1+ X_2W_2+ X_3W_3+.....+ X_mW_m$

i.e$Y_{in}=\sum_1^m X_iW_i$

Where X_1, X_2 ... X_m are input signals and W_1, W_2..... W_m are strength of synapse which are connected to input signals to neuron. The neurons are the processing unit which will calculates the weighted sum of the input.

MFCC

The 5th processing step is the Mel frequency spectrum. Where the Mel frequency spectrum is filtered with different band pass filters and the power of each spectral band weight calculated or computed. The computed filter banks applying to angular filters. The main scale aims to mimic the normal human ear perception bye low frequency discriminative and is at higher frequency is less discriminative. We can convert frequency and Mel spectrum (m) using the below equations

$m=2595\log_{10}(1+ (f/700))$

$f=700(10^{(m/2595)}-1)$

Windowing

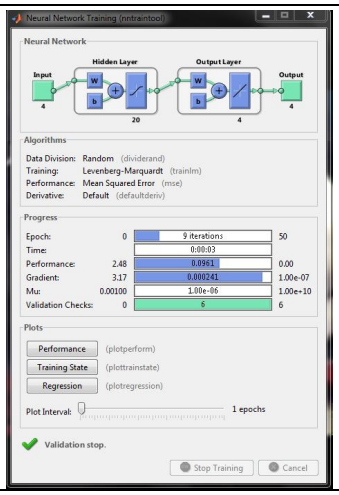
In signal processing the window function plays an important role. It is also called as function where zero valued outside of the interval normally symmetric around the middle bandwidth. In this process the waveform of the speech signal is multiplied with window function (hamming function). The modelling is done by multiplying buy one inside the window and outside the window.

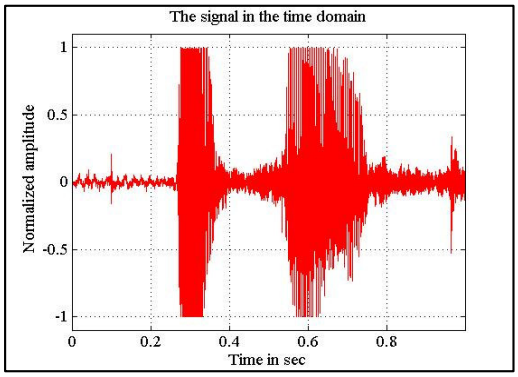
Frame Blocking Windowing

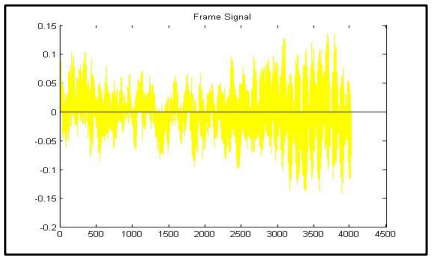
The speech signal is divided into a sequence of frames where each frame can be analyzed independently and represented by a single feature vector. Since each frame is supposed to have stationary behaviour, a compromise, in order to make the frame blocking, is to use a 20-25 ms window applied at 10 ms intervals (frame rate of 100 frames/s and overlap.) In order to reduce the discontinuities of the speech signal at the edges of each frame, a tapered window is applied to each one. The most common used window is Hamming window, described as below

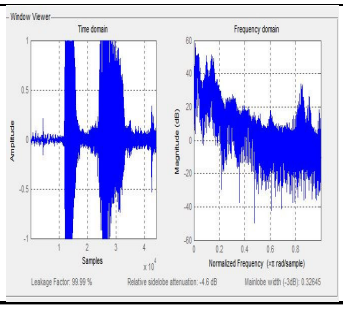
RESULT

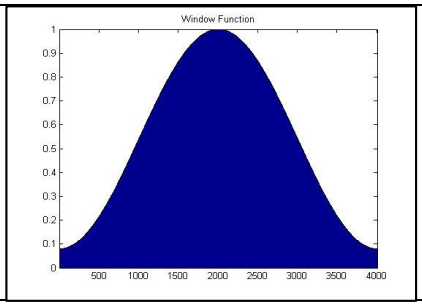
NEURAL NETWORK TRAINING

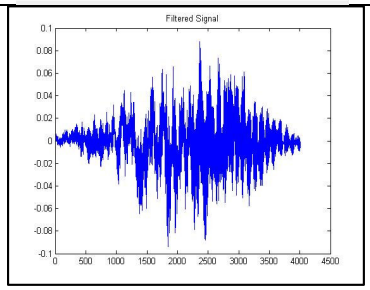

Neural Network Training (nntraintool)
Neural Network
Hidden Layer
Output Layer
Input
Output
Algorithms
Data Division: Random (dividerand)
Training: Levenberg-Marquardt (trainlm)
Performance: Mean Squared Error (mse)
Derivative: Default (defaultderiv)
Progress
Epoch: 0 9 iterations 50
Time: 0:00:03
Performance: 2.48 0.0961 0.00
Gradient: 3.17 0.000241 1.00e-07
Mu: 0.00100 1.00e-06 1.00e+10
Validation Checks: 0 6 6
Plots
Performance (plotperform)
Training State (plottrainstate)
Regression (plotregression)
Plot Interval: 1 epochs
Validation stop.
Stop Training
Cancel

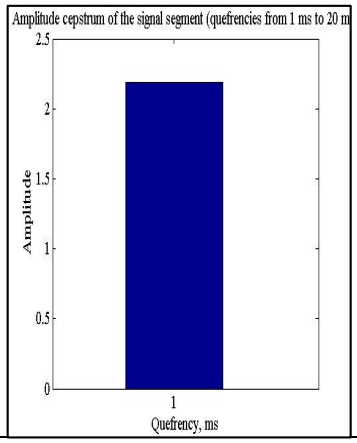

The signal in the time domain
Normalized amplitude
Time in sec


Frame Signal


Window Viewer
Time domain
Frequency domain
Amplitude
Magnitude (dB)
Samples
Normalized Frequency (×π rad/sample)


Window Function


Filtered Signal


Amplitude cepstrum of the signal segment (quefrencies from 1 ms to 20 m
Amplitude
Quefrency, ms

CONCLUSION

From the presented work, it is concluded that neural networks can be very powerful models for the classification of speech signals. Some types of very simplified models can recognize the small set of words. The performance of the neural networks is being impacted largely by the pre- processing technique. On the other hand, it is observed that Mel Frequency Cestrum Coefficients are very reliable tool for the pre-processing stage. Very good results are provided by these coefficient

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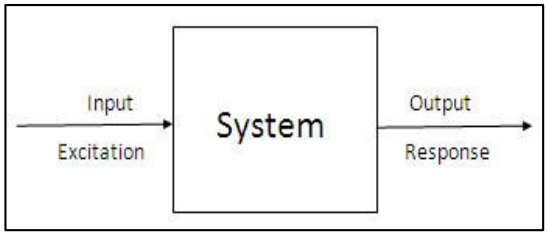

Fig1-Simple system

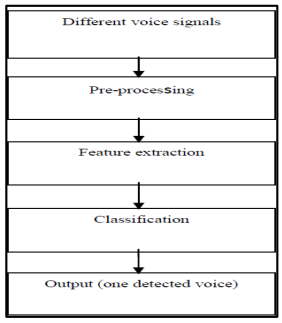

Fig-2 Speech Recognition Using Ann Method

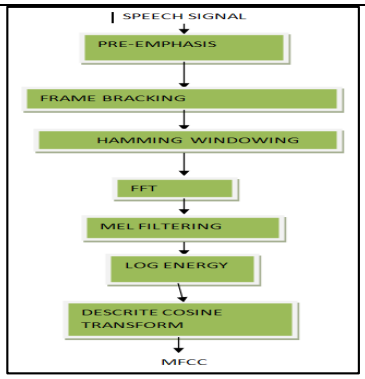

Fig3:MFCC

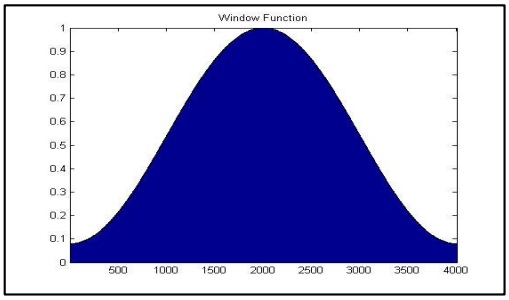

Fig.4 Windowing

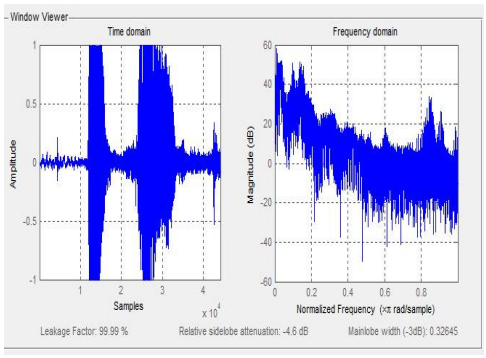

Fig.5 Frame Blocking Windowing

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REVIEW ARTICLE

Review of Different Techniques for Classifying and Retrieving the Data from Big Data

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ABSTRACT

Big Data is term for datasets that are so large or complex that the traditional data processing application software is inadequate. The use of Big Data has widely spread during the recent times. All the multimillion companies has started implementing methods to make the best use of it. Big Data has its own share of challenges to be dealt with. As the data is really large the retrieving of useful information and classifying the data is a huge challenge.The software experts strived hard in developing the algorithms for classifying and retrieving the data required. The retrieving is dependent on queries produced by the user.

Keywords: Big Data, Data sets, Classification

AIM

The aim of our paper is the software experts strived hard in developing the algorithms for classifying and retrieving the data required. The retrieving is dependent on queries produced by the user. In our project we implement a classification algorithm called KNN (K Nearest Neighbors) that classifies the data and gives a map of the nearest neighbors.

History

Big data is a term for data sets that are so large or complex that traditional data processing application software is inadequate to deal with them. Challenge includes capture, storage, analysis, data curation, and search, sharing, transfer, visualization, querying, updating and information privacy. The term "Big Data" often refers simply to the use of predictive analysis, user behaviour analytics, or certain other advanced data analytical methods that extract value from data, and seldom to a particular size of the data set. There is little doubt that the quantities of data now available are indeed large, but that's not the most relevant characteristic of this new data ecosystem. Analysis of data sets can find new correlations to "spot business trends, prevent diseases, and combat crime. Scientists, business

executives, practitioners of medicines, advertising and governments alike regularly meet difficulties with large data sets in areas including internet search, finance, urban informatics and business informatics.

Description

Data sets grow rapidly – in part because they are increasingly gathered by information-sensing mobile devices, aeriel (remote sensing), software logs, cameras, microphones, Radio Frequency Indentification (RFID) readers and wireless sensor networks. The world's technological per-capita capacity to store information has roughly doubled every 40 months since the 1980s; as of 2012, every day 2.5 extrabytes (2.5×10^{18}) of data are generated. One question for large enterprises is determining who should own big-data initiatives that affect the entire organization. Relational database management systems and desktop statistics- and visualization-packages often have difficulty handling big data. The work may require "massively parallel software running on tens, hundreds, or even thousands of servers". What counts as "big data" varies depending on the capabilities of the users and their tools, and expanding capabilities make big data a moving target. "For some organizations, facing hundreds of gigabytes of data for the first time may trigger a need to reconsider data management options. For others, it may take tens or hundreds of terabytes before data size becomes a significant consideration."

Motivation

The computing revolution that began more than two decades ago has led to large amounts of digital data being amassed by corporations. Advances in digital sensors; proliferation of communication systems, especially mobile platforms and devices; massive scale logging of system events; and rapid movement toward paperless organizations have led to a massive collection of data resources within organizations. And the increasing dependence of businesses on technology ensures that the data will continue to grow at an even faster rate.

Purpose

The concept of Big Data has been around for more than a decade – but while it is potential to transform the effectiveness, efficiency, and profitability of virtually any enterprise has been well documented, the means to effectively leverage Big Data and realize its promised benefits still eludes some organizations. Ultimately, there are two main hurdles to tackle when it comes to realizing these benefits. The first is realizing that the real purpose of leveraging Big Data is to take action – to make more accurate decisions and to do so quickly. We call this situational awareness. Regardless of industry or environment, situational awareness means having an understanding of what you need to know, what you have control of, and conducting analysis in real-time to identify anomalies in normal patterns or behaviors that can affect the outcome of a business or process. If you have these things, making the right decision within the right amount of time in any context becomes much easier.

Scope

A team of statisticians, data scientists and software engineers experienced in handling big data platforms such as Hadoop, MongoDB etc. Inclusion of data from social media and other publicly available sources for better insights and decision making. Integration of Sentiment Analysis engine with Big Data platform to process large volumes of data from internal as well as publicly available sources.

LITERATURE SURVEY

The aim of this section is to provide a review of the research efforts related to effective temperature monitoring systems.

Big Data

The term has been in use since the 1990s, with some giving credit to John Masheyfor coining or at least making it popular. Big data usually includes data sets with sizes beyond the ability of commonly used software tools to

capture, curate, manage, and process data within a tolerable elapsed time. Big data "size" is a constantly moving target, as of 2012 ranging from a few dozen terabytes to many petabytes of data. Big data requires a set of techniques and technologies with new forms of integration to reveal insights from datasets that are diverse, complex, and of a massive scale.

In a 2001 research report and related lectures, META Group (now Gartner) defined data growth challenges and opportunities as being three-dimensional, i.e. increasing volume (amount of data), velocity (speed of data in and out), and variety (range of data types and sources). Gartner, and now much of the industry, continue to use this "3Vs" model for describing big data. In 2012, Gartner updated its definition as follows: "Big data is high volume, high velocity, and/or high variety information assets that require new forms of processing to enable enhanced decision making, insight discovery and process optimization." Gartner's definition of the 3Vs is still widely used, and in agreement with a consensual definition that states that "Big Data represents the Information assets characterized by such a High Volume, Velocity and Variety to require specific Technology and Analytical Methods for its transformation into Value". Additionally, a new V "Veracity" is added by some organizations to describe it, revisionism challenged by some industry authorities. The 3Vs have been expanded to other complementary characteristics of big data.

Volume: big data doesn't sample; it just observes and tracks what happens
Velocity: big data is often available in real-time
Variety: big data draws from text, images, audio, video; plus it completes missing pieces through data fusion
Machine learning: big data often doesn't ask why and simply detects patterns

Digital footprint

big data is often a cost-free byproduct of digital interaction. The growing maturity of the concept more starkly delineates the difference between big data and business intelligence Business Intelligence uses descriptive statistics with data with high information density to measure things, detect trends, etc. Big data uses inductive statistics and concepts from nonlinear system identification to infer laws (regressions, nonlinear relationships, and causal effects) from large sets of data with low information density to reveal relationships and dependencies, or to perform predictions of outcomes and behaviors.

Advantages

Big Data is Timely –60% of each workday, knowledge workers spend attempting to find and manage data.
Big Data is Accessible –Half of senior executives report that accessing the right data isdifficult.
Big Data is Holistic –Information is currently kept in silos within the organization.Marketing data, for example, might be found in web analytics, mobile analytics, social analytics, CRMs, A/B Testing tools, email marketing systems, and more each with focus on its silo.
Big Data is Trustworthy –29% of companies measure the monetary cost of poor dataquality. Things as simple as monitoring multiple systems for customer contact information updates can save millions of dollars.
Big Data is Relevant –43% of companies are dissatisfied with their tools ability to filter outirrelevant data. Something as simple as filtering customers from your web analytics can provide a ton of insight into your acquisition efforts.
Big Data is Secure –The average data security breach costs $214 per customer. The secureinfrastructures being built by big data hosting and technology partners can save the average company 1.6% of annual revenues.
Big Data is Authoritative –80% of organizations struggle with multiple versions of the truthdepending on the source of their data. By combining multiple, vetted sources, more companies can produce highly accurate intelligence sources.

Big Data is Actionable –Outdated or bad data results in 46% of companies making baddecisions that can cost billions.

Applications

- Health Care
- Education
- Media
- Manufacturing
- Internet of Things(IOT)
- Retail

Description

Big Data is a phrase used to mean a massive volume of both structured and unstructured data that is so large that it is difficult to process using traditional database and software techniques. In most enterprise scenarios the volume of data is too large or too fast as it exceeds current processing capacity. Big Data has the potential to help companies improve operations and make faster, more intelligent decisions. This data, when captured, formatted, manipulated, stored and analysed can help a company to gain useful insight to increase revenues, get or retain customers and improve operations. Big data is the term that may seem to reference volume of data. But in case of vendors, it may refer to technology that an organization required to handle the amounts of data and storage. The technology consists of tools and processes.

Volume: Organizations collect data from a variety of sources, including business transactions, social media and information from sensor or machine-to-machine data. In the past, storing it would have been a problem – but new technologies (such as hadoop) have eased the burden.

Velocity: Data streams in at an unprecedented speed and must be dealt with in a timely manner. RFID tags, sensors and smart metering are driving the need to deal with torrents of data in near-real time.

Variety: Data comes in all type of formats from structured, numeric data in traditional databases to unstructured text documents, email, video, audio, stock ticker data and financial transactions.

Variability: In addition to the increasing velocities and varieties of data, data flows can be highly inconsistent with periodic peaks. Is something trending in social media? Daily, seasonal and event-triggered peak data loads can be challenging to manage.

Complexity: Data comes from multiple sources, which makes it difficult to link, match, cleanse and transform data across systems. However, its necessary to connect and correlate relationships, hierarchies and multiple links or your data can quickly spiral out of control.

Potential: As the data keeps growing day by day the need for big data keeps raising. The data on global level is almost inconceivable and it keeps growing. It is estimated that all the information the world has acquired till 2013 is equal to the amount that we got in the next two years. The big data has the potential to store, search and retrieve all this information to us. It is probably the only source in the world right now that can help us the growing data.

It can be embedded with the latest technologies like IOT, Neural Networks to get the better results. The data we receive has already been revolutionized during the recent times by developing the means of social networking and it can only get better with big data.

Review on Big Data

In the current scenario, Web and its associated entity, Internet, a shadow has been cast on the same with the data explosion that has taken place in the last couple of years considering the interaction that has been taking place between people and systems associated at multiple touch points. This huge entity which is taking place at every touch point as mentioned above in its wholesome behaviour is known as Big Data. Some decades earlier, Kilobytes and Megabytes used to be entities, which used to combine the entire definition of data existing on the planet, and due to continuous interactions between people and systems that have been taking place which has lead to exponential growth of data due to which new terms such as Gigabytes, Terabytes, Petabytes, Exabyte's & Zettabytes have graced the steps of the computing world. Theorists and Researchers have propagated this that as Moore's law was to growth of transistors inside the circuits, Data in Internet would exceed the entire brain capacity of the living species. Technological advances have been taking place continuously across all the domains and the major reasons for it are advances in digital sensors, computation, communications and storage that have created humongous collection of data.

As explained above, data is generated through various sources which will be used by multiple organizations to run and understand the various business scenarios which help them understand and run their business. All the above data when analysed through various sources and methods of data analysis help organizations in studying customer behaviour, interpreting market trends and taking strategic and financial decisions. When we speak about Big Data, as we have done above, we often identify it as a jargon, catch phrase which means a exponential volume of unstructured and structured data that contains so many huge datasets which cannot be processed by traditional database management techniques and associated software techniques. With the size of the big data and simply the capacity of the data that it encompasses, it carries in itself the potential that will help companies, in making far better, intelligent and data driven decisions and help in improving operations. For most of the organizational scenarios, it can be easily identified either the data is in excess of the current storage and processing capacity, or the volume of the data is too big or it moves too fast. To give insights using the same data, that we have spoken about earlier, it has to help us in giving insights which would help us in gain competitive advantage, increasing revenues and customer retention and for that we need to capture the data, clean the data, format, manipulate, store and analyze the same.

Data Forms

Structured

When we talk about structured data, we often conclusively identify that, as soon as we placed our current data ware house in the relational database management system, the structure of the relational database management system was enforced on the current data ware house system, which is inclusive to understand the meaning associated with it. So we know, which columns are placed where, whom are they associated with and how the columns are associated in between tables and table spaces. The format of the data can be in text or numerical, but it is common understanding that for every person there is a unique identifier in terms of Age.

The entire data is organized in terms of Entities (Semantic Chunks).

Relations or Classes (Similar entities are grouped together).

Attributes (Same descriptions for entities existing in the Same groups)

Schema (All Entities in the group have a description associated with it.

Semi Structured

As we move on from structured data to semi structured data, there is little to demarcate and often the differentiating lines goes blurry. The data format that we are describing here does not conform to an explicit and fixed schema, however the tags associated with the data, if found associated with organizational structure, then the same data would be easier to analyze and organize. The same concept described here would predate the idea of XML but not HTML. Data is available in many formats, in the current scenario, electronically

- Database Systems
- File Systems e.g., Bibliographic data, Web data
- Data Exchange Formats, e.g. EDI, Scientific data
- Data that is not completely structured, but partially as spoken earlier
- Grouping of Similar Entities and semantically organized
- Entities may not have same attributes in the group

Unstructured

We have already discussed about the Structured and Semi Structured formats. Moving on to the unstructured format, this type would consists of formats that cannot be easily indexed. When we talk about indexing, it is with reference of relational tables and for the purpose of querying or analysis. This would include the file types that are associated with audio, video and image files.

Importance of Big Data

Importance would be defined in terms of how effective this concept has been for organizations, in improving their most important KPI's, also not with the quantity of data the organization has, but with the insights that it has helped to generate. Data is taken from multiple source and integrated across various environments which when analyzed can help us give answers to following:

- Time & Cost reductions.
- Customized & Optimized Market Offerings & New Product Development.
- Strategy Development & Smart Decision Making.

In a Business environment, there are a lot of decisions that are to be taken on the basis of Data & associated analytics and in simple terms, we could define it as Big Data when combined with powered analytics, lot of business related tasks can be accomplished such as:

- Root Cause Analysis can be conducted in real time for associated defects, failures and issues.
- POS based generated coupons based on Consumer Behaviour.
- Risk Portfolio – Quick Calculations/Re-Calculations can be conducted in minutes.
- Conducting Fraud Detection & use of Fraud analytics before hitting organization.

Big Data Characteristics

As mentioned before, big data is a concept and the same can be defined through a model and in our case, it can be defined through 3V model, whose definition was casted by Laney, "high-volume, high-velocity and high-variety information assets that demand cost-effective, innovative forms of information processing for enhanced insight and decision making". Recently in 2012, Gartner processed the definition of Big Data as "Big data is high volume, high velocity, and/or high variety information assets that require new forms of processing to enable enhanced decision making, insight discovery and process optimization". By definitions, both aforementioned incorporate three main features: Volume, Variety, and Velocity. When the concept is spread across organizations and different business models & big data practitioners, the 3V model can be extended to 4V (V for Value added) or 5V (V for Veracity) could be another factors dependent on the organization, which model they want to adapt. Getting a summary of the same, we can easily state that these models, provide a straightforward and all accepted definitions related to what all is incorporated in a big data based application, solution, problem and framework.

Volume: This would refer to the data from multiple sources, data being in huge capacity. It caninclude all and any kind of data, including the data that is created from all the connected devices, IoT & mobile data and all the data that is being resulted from this communication. In the current scenario, it can be easily stated that, data that is being generated is being approached in computer memory sizes, that were being heard of exabytes, petabytes & zettabytes. It will be coined to reach terms, that are still undefined and new names would have to be though for the same. However, since the data is being generated at the capacity, that we are unable to comprehend, and organizations are still trying to keep up with that pace. Consequences, that are being resulted from these actions, it has become anormalcy for the companies, to store enormous and varied amounts of data : financial, biochemistry, electronics, computer records, genetic, social networks & healthcare. The benefits that are being generated from incorporating this data, are companies at their disposal have a lot of data, which is a challenges in itself, however, valuable information can be obtained from the same regarding people & companies.

Velocity: When we talk about transferring a movie, than we really do not worry about velocity, forthat movie will be approximately 1 Gigabyte in size and would take a minute to complete. But when we talk about the big data, we can easily state that, for the data that is of the size of exabytes & petabytes, the same data, would take a lot of time to transfer and hence the velocity becomes a very important factor as it affects performance also. When we speak about the data, the contents are constantly changing, via introduction of previous or legacy collections & absorption of complementary data collections and will involve data streamed through multiple sources. Velocity not only involves, the speed at which the data is transferred, but will also involve, data streams, creation of structured records, access to data & delivery. The issues does not only lie with the velocity of incoming data but also to stream outgoing data for batch processing.

Variety: This refers to varied data types and the same can be accumulated from various sources,sources being: social networks, Smartphone, sensors in the forms of videos, images, audio, logs etc. This data can be highly structured (data fetched from the traditional database systems), semi-structured (feeds – social, rss, raw; web logs) or unstructured (clicks, audio, images, videos).

Value: It refers to the critical & valuable information that is being extracted from big datasets thatare associated with the concept of Big Data and this concept in its entirety is called as Big Data Analytics. When we speak about the 4V model, V that stands for Value becomes the most critical factors for any Tanvi, Dr. Radha Krishna Page 26 application based on Big Data & this for the sole reason that it allows to generate useful business information. Till recent times, large volumes of data were recorded as part of regulations but never analysed or exploited. Considering that fact, Value is highly subjective in nature. Big Data as a concept brings with itself the technologies, that enables people & organizations to help exploit the data, the way it was never done before.

Veracity: This term would refer to the accuracy & correctness of the data on which the analysis is tobe conducted. A lot of uncertainties can be caused for the most simple of reasons such as : Data inconsistency, Data Ambiguity, Data Duplications, incompleteness, deception, fraud, duplication, Approximated models, spam & latency. It is not necessary, that the analysis on top of big data, would give a perfect conclusive result. However, everything can be assigned a probability.

Analysis on Big Data

Data Acquisition and Recording

After discussing so much on Big Data, we can safely assume that,Big Data does not simply appear out of thin air. There are multiple sources from which data is recorded. Since we are accumulating so much data, it will be obvious, that part of the data will be of no use & speaking in that way, filtering & compression techniques can be used to sort the matter out. When speaking out about filtering & compressing, we have to take care to define them in such a way,

that they should not leave out important information. The other challenge that we would be speaking about is the generation of right metadata to describe the recording of the data and measurement of the same. Also, at the same point of time, we can easily state that, recording the information about the data at the start/birth is not useful since in the pipeline it will keep on changing and interpreted in different ways while being carried through the data analysis stages.

Information Extraction and Cleaning

Simply collecting the information would not help ingenerating analysis or will not be in a state to generate analysis and insights. Data simply in this collected form, will not be in a format which can be analysed. To do this correctly, we need a process which will help us in extracting information, that will help us in pulling out the required information and will be presented in a structured analysis, which will help us in generating insights from the same. Doing the aforementioned process again and again, and that too in a continual manner with correctness being the top priority is a technical challenges that is continuous in nature. Data cleaning is one of the primary focus areas, that assumes constraints that are well documented and well recognized on valid data or error models that have a deep understanding with reference to the data. For most of the areas, where Big Data emergence is new, these models do not exist.

Data Integration, Aggregation, and Representation

When we speak on the current topic, wewould be talking about Data analysis. Data Analysis is not as simple as the meaning it connotates, for it includes challenges than simple location, identification, understanding & citing data. When we speak about the analysis that is constituted on a large scale, it would be happening in a purely automated fashion. In the current scenario, when we speak about Database Design, it is an art as opposed to science. When we speak about the aforementioned top heroic as science, it has to be developed in a context, whether it being in the Enterprise or Cloud context. Domain Scientists has emerged as a new context, where in they are highly paid professionals along with enabling other professions in the same domain as well, to develop effective database designs. These can be achieved via various ways: design process will be assisted by devising tools, revamping the designing process, development of new techniques and all of them will be used for effective creation of intelligible database design.

Query Processing, Data Modeling, and Analysis

Big data is traditionally different from traditionaldatabase management systems and hence the methods for querying & mining in Big Data are different from traditional statistical techniques which will be different on Big & small samples. When we talk about Big Data, we often associate it with being dynamic, inter-relationships, untrustworthy & noisy as opposed to the process of mining, which will require clean, trustworthy, integrated, efficient, accessible data which can be accessed via mining interfaces using declarative queries, scalable mining algorithms and computing environments for big data. When we are speaking of the aforementioned topics, we can easily state that the data mining itself can be used to help with trust quotient of data as well improving quality of the same, understanding the associated semantics of the data & provide insightful & intelligible querying functions. One of the major problem that Big Data faces is that there is no coordination between the database packages which host the big datasets that are part of the Big Data. Part of the Database systems host the data, part deal with SQL Querying and other ones host the data mining and statistical analysis.

Interpretation

We should understand that analysis is of limited value, if user cannot understand thesame with reference to Big Data. Even if analysis is done all the reports and graphs are generated, one still has to sit and interpret the same. The interpretation cannot happen, while sitting alone in a cubicle or vacuum as the person analysing the reports and graphs has to take care of the assumptions that were used while generating the analysis and retracing the steps.

Big Data Ecosystem

While speaking about the Big Data, we can sense that and would like to statethat, it is a problem, not only related to database or Hadoop, but would constitute technologies at its core and components for data processing on large scale and data analytics. The entire structure of components to analyze by storing, processing, visualizing and delivering results to applications which were the target incorporating Big Data as "fuel" for all the processes which are data related and associated source, target and outcome. All the associations between the components and the intertwined relationships can be incorporated into the BDE or Big Data Ecosystem that will incorporate in itself all the data, supporting infrastructure, models during entire Big Data Lifecycle.

Techniques and Technologies

In the current paper, we will not be giving an in depth overview on the tools and techniques, however, we will be giving an overview of the tools and techniques associated with Big Data. This will help the reader get a association with the tools used for Big Data analytics.

Techniques

There are a lot of techniques that could be used when going to start with a project. Some of the tools which have frequent usage are summarized here.

Association rule learning

A set of techniques for discovering interesting relationships, i.e.,"association rules," among variables in large databases.

Data mining

One of the most important terms related to data-driven decision making and describesit as "searching or 'digging into' a data file for information to understand better a particular phenomenon."

Cluster analysis

Cluster analysis is a type of data mining that divides a large group into smallergroups of similar objects "whose characteristics of similarity are not known in advance."

Crowd sourcing

Crowd sourcing collects data from a large group of people through an open call,usually via a Web2.0 tool. This tool is used more for collecting data than for analyzing it.

Machine learning

Traditionally computers only know what we tell them, but in machine learning, asubspecialty of computer science, we try to craft "algorithms that allow computers to evolve based on empirical data.

Text analytics

A large portion of generated data is in text form. Text Analytics is the process ofconverting unstructured text data into meaningful data.

Technology

As with the analytical techniques, there are several software products and availabletechnologies to facilitate big data analytics. Some of the most common will be discussed here.

EDWs: Enterprise data warehouses are databases used in data analysis.

Visualization products

One of the difficulties with big data analytics is finding ways to visuallyrepresent results. Many new visualization products aim to fill this need, devising methods for representing data points numbering up into the millions. Beyond simple representation visualization can also help in the information search.

MapReduce

MapReduce is a processing technique and a program model for distributed computingbased on java. The MapReduce algorithm contains two important tasks, namely Map and Reduce. Map takes a set of data and converts it into another set of data, where individual elements are broken down into tuples (key/value pairs). Secondly, reduce task, which takes the output from a map as an input and combines those data tuples into a smaller set of tuples.

Hadoop

It is an open-source framework that allows to store and process big data in a distributedenvironment across clusters of computers using simple programming models. Hadoop is an Apache managed software framework derived from MapReduce and Big Table.

NoSQL databases

NoSQL database, also called Not Only SQL, is an approach to data managementand database design that's useful for very large sets of distributed data. NoSQL is especially useful when an enterprise needs to access and analyze massive amounts of unstructured data or data that's stored remotely on multiple virtual servers in the cloud. The most popular NoSQL database is Apache Cassandra. Other NoSQL implementations include SimpleDB, Google BigTable, Apache Hadoop, MapReduce, MemcacheDB, and Voldemort.

Usage Areas of Big Data

Big data is used efficiently in numerous fields. Some of them are listed below:

- Automotive industry
- High technology and industry
- Oil and gas
- Telecommunication sector
- Medical field
- Retail industry
- Packaged consumer products
- Media and show business
- Travel and transport sector
- Financial services
- Social media and online services
- Public services
- Education and research
- Health services
- Law enforcement and defense industry

SUMMARY

Big Data is the latest technology that stores, searches and retrieves the data for the end user.The tools and software for using this technology are being developed in the recent times by most of the multi-million companies.Our project is an effort that we did in this field using the K-means methods which is an algorithm that is being used in Big Data.

CONCLUSION

After writing this report/paper, we have developed better understanding of this concept called as Big Data after we have been able to put words to it. We have been able to define models, ecosystems and categorize elements on the basis of it. We also have been able to identify the tools and techniques that have been associated with Big Data Analytics on a frequent basis. On the basis of the analysis conducted, we identified the areas with maximum usage of Big Data Analytics.

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RESEARCH ARTICLE

Effect of Current and Pulse Time for Machining Alluminium, Brass, Stainless Steel, Mild Steel and En8 Byelectro Discharge Machinig

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ABSTRACT

Electric discharge machining (EDM) is one of the most efficient non-conventional manufacturing technologiesused in highly accurate processing of all electrically conductive materials irrespective of theirmechanical properties. It is a non-contact thermal energy process applied to a wide range ofapplications, such as in the aerospace, automotive, tools, molds and dies, and surgical implements,especially for the hard-to-cut materials with simple or complex shapes and geometries.This present work represents the variation of machining parameters (current, pulse on time, pulse off time and machining time) in EDM on machining performance (MRR and surface roughness) of aluminum, brass, mild steel (MS), stainless steel (SS) and EN8. The result provides a better comparative conclusion among the parameters on their performances in EDM.

Key words: EDM, Pulse on Time, Pulse off Time, MRR, Surface Roughness.

INTRODUCTION

In recent years, rapid developments in aerospace, medical instruments, transportation, and many other industrial sectors increased the need for new materials with favorable characteristics. In additionto unique characteristics, most modern materials need special manufacturing processes to enable themto be machined with ease [1,2]. Most of these materials are usually diffiult to cut by conventionalmanufacturing processes [3–5]. The unique characteristics of these hard-to-cut materials increase theirapplications, which further drive manufacturers to explore new machining processes with reasonablecost and high precision [6]. Electric discharge machining (EDM) is one of the most advanced manufacturing methods used to successfully machine conductive hard-to-cut materials [7-9]. EDM is the

process of choice tomachine hard-to-cut materials widely used in modern industries to facilitate accurate machining [10-11], complex shape machining, and better surface integrity. The process is utilized to machine electricallyconductive materials by applying repetitive sparks between electrode and workpiece. Unlike inmechanical machining, no deforming force is required between the electrode and the workpiece, andthe machining takes place without actual contact between them [12-13]. There are a large numberof variants of the EDM process such as sinking EDM, wire EDM, micro-EDM, powder-mixed EDM,and dry EDM; all of these possess work on the same mechanism of material removal. EDM can be used to machine the materials which have complex shape and size. Since there isno direct contact between the electrode and work piece, so there are no mechanical energyexisting between them. Any type of electrically conductive hard materials can be machinedby EDM irrespective of the hardness or toughness of the material.

Experimental Work

To determine the effect of Current and Pulse Time for machining of Aluminum, Brass, Stainless Steel, Mild Steel by an Electron Discharge Machine (EDM), so as to find out the optimum input parameters which will enable minimum machining time while maintaining an acceptable surface roughness. Four samples from each of the five materials were taken, the images of which are shown below.Each of the samples were of cylindrical shape with diameter of 40mm and thickness of 15mm.Then each of the four samples from each of the five materials were machined by providing randomly chosen 4 combinations of input parameters and the Output parameters were recorded as in the following tables.

RESULTS AND DISCUSSION

After the experimental procedures, the performance parameters were taken out and recorded as shown in tables 1,2,3,4 and were compared from which the following remarks were analyzed.

CONCLUSIONS

From the above experiment and analysis, the followings may be concluded.

1. The surface roughness of machined workpieces significantly increases with higher values of machining parameters i.e. pulse on time, pulse off time, duration of machining significantly. However, for better surface finish, the values of input parameters should be imposed in a controlled manner which may lead to significant improvement in performance parameter.
2. It was also obvious to state that, the rate of material removal (MRR) also increases with the increase in input parameters which is significant about the statement regarding surface roughness values of workpieces. However, the values of machining input parameters may be selected keeping in views the responses and utilization of performance parameters.

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Table 1: Machining Parameters & Performances of sample 1.

Sample No.	Material	Initial Wt. (gm)	Final Wt. (gm)	Current (Amp)	(T)On (Sec.)	(T)Off (Sec.)	M/C Time (Sec.)	MRR (gm/hr.)	Surface Roughness (μm)
1	Aluminum	39.6	34.4	3	50	5	57.65	5.412	1.273
	Brass	179.9	178.5	3	50	5	104.7	0.802	1.087
	MS	166.6	165.4	3	50	5	73.45	0.980	2.680
	SS	154.1	153.1	3	50	5	66.33	0.905	2.543
	EN8	188.2	186.9	3	50	5	73.78	1.057	2.710

Table 2: Machining Parameters & Performances of sample 2.

Sample No.	Material	Initial Wt. (gm)	Final Wt. (gm)	Current (Amp)	(T)On (Sec.)	(T)Off (Sec.)	M/C Time (Sec.)	MRR (gm/hr.)	Surface Roughness (μm)
2	Aluminum	33.6	33.2	5	150	15	19.65	1.221	1.887
	Brass	185.5	184.4	5	150	15	46.52	1.419	1.717
	MS	161.1	159.6	5	150	15	37.98	2.370	3.913
	SS	163.8	162.5	5	150	15	28.75	2.713	3.763
	EN8	184.8	183.5	5	150	15	33.40	2.335	4.390

Table 3: Machining Parameters & Performances of sample 3.

Sample No.	Material	Initial Wt. (gm)	Final Wt. (gm)	Current (Amp)	(T)On (Sec.)	(T)Off (Sec.)	M/C Time (Sec.)	MRR (gm/hr.)	Surface Roughness (μm)
3	Aluminum	36.4	36.2	7	100	10	7.37	1.628	3.110

	Brass	169.8	168.5	7	100	10	32.57	2.395	1.770
	MS	172.6	171.3	7	100	10	19.33	4.035	4.023
	SS	170.7	169.7	7	100	10	14.10	4.255	3.850
	EN8	158	156.7	7	100	10	17.77	4.389	4.867

Table 4: Machining Parameters & Performances of sample 4.

Sample No.	Material	Initial Wt. (gm)	Final Wt. (gm)	Current (Amp)	(T)On (Sec.)	(T)Off (Sec.)	M/C Time (Sec.)	MRR (gm/hr.)	Surface Roughness (μm)
4	Aluminum	37.9	37.6	10	250	20	3.22	5.590	5.053
	Brass	174.6	173.1	10	250	20	15.70	5.732	2.573
	MS	167	165.8	10	250	20	10.12	7.115	6.113
	SS	148.4	147.1	10	250	20	10.70	7.290	4.953
	EN8	180.3	179.1	10	250	20	11.57	6.223	3.945

Figure 1: Specimen Samples.

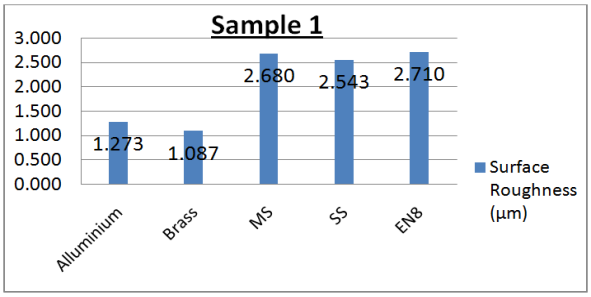

Figure 2: Surface Roughness Comparison for sample 1.

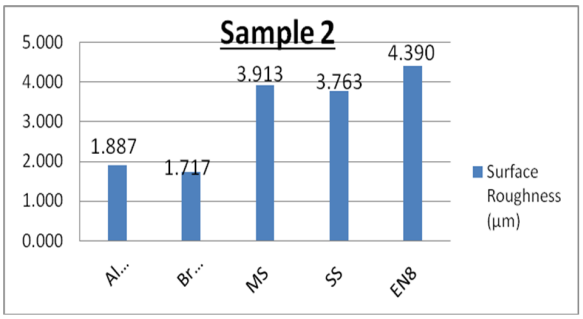

Figure 3: Surface Roughness Comparison for sample 2.

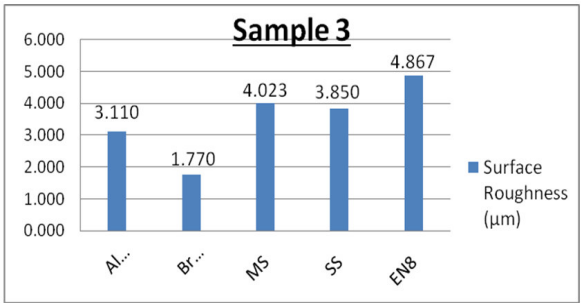

Figure 4: Surface Roughness Comparison for sample 3.

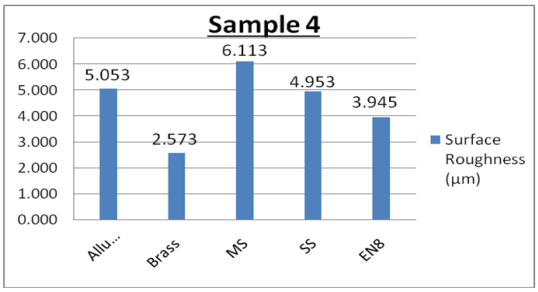

Figure 5: Surface Roughness Comparison for sample 4.

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RESEARCH ARTICLE

Numerical Analysis of Fatigue Damage Development for Braided Carbon-Fiber Polymer Matrix Composite

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ABSTRACT

In this present work, a review of the major fatigue models and life time prediction methodologies for fiber-reinforced polymer composites subjected to fatigue loadings has been studied. A composite plate is modelled having a centre hole and four holes on each corner of the plate. For conducting this fatigue damage analysis validation, a comparison is done with available literature, which shows good agreement. Further fatigue damage analysis has been carried out on a braided carbon fiber composite plate with different material parameters. A three-dimensional finite element method has also been followed using FE Software (ANSYS 19) for the analysis of fatigue damage evaluation of both materials i.e. structural steel and braided carbon fiber polymer matrix composite material. The results have been compared with the fatigue damage behaviour of structural steel and composite material & found that the strength and the load bearing capability of a braided type composite material has much greater than that of the conventional materials .

Keywords: Composite material, Braided type composite material, Fatigue Analysis, Finite Element Method.

INTRODUCTION

Composites are combinations of two materials in which one of the materials, called the reinforcing phase, is in the form of fiber sheets or particles and are embedded in the other material called the matrix phase. The primary functions of the matrix are to transfer stresses between the reinforcing fibers/particles and to protect them from mechanical and/or environmental damage whereas the presence of fibers/particles in a composite improves its

mechanical properties such as strength, stiffness etc. A composite is therefore a synergistic combination of two or more micro-constituents that differ in physical form and chemical composition and which are insoluble in each other. Fiber reinforced polymer composites are now considered as an important class of engineering materials. They offer outstanding mechanical properties, unique flexibility in design capability and ease of fabrication. Additional advantages include light weight, corrosion and impact resistance and excellent fatigue strength. Today, fiber composites are routinely used in such diverse applications as automobiles, aircraft, space vehicles, off-shore structures, containers and piping, sporting goods, electronics and appliances. A fiber reinforced composite is not simply a mass of fibers dispersed within a polymer.

It consists of fibers embedded in or bonded to a polymer matrix with distinct interfaces between the two constituent phases. The fibers are usually of high strength and modulus and serve as the principal load carrying members. The matrix acts as the load transfer medium between fibers and in less ideal cases where loads are complex, the matrix may even have to partly bear loads. The matrix also serves to protect the fibers from environmental damage before, during and after composite processing. The carbon fiber Reinforced polymer matrix material or CFRP is the type of composite material in which the composite consists of two parts: one is matrix and another part is reinforcement where carbon fiber is used as reinforcement which provides the high or good strength and the matrix is usually as a polymer resin, such as epoxy. The braided type of composite materiala are mostly used now a days in various fields because of their superior strength &high stress bearing capacity.

The main motive to use this braided type composite materials are, Generally, when a structure is relative to elevated fatigue load or fatigue cycles, there are some micro-cracks occurs direction of the matrix of prep rag laid-up structures. So the micro-cracking can be minimized at the yarns of intersections of the reinforcing, so that this material can be easily adapted in the aerospace industry. Its impact resistance enhanced during efficient distribution of the load in a braided structure. Numerous experimental as well as computational studies have been developed to investigate the fatigue damage development. With their high stiffness-to-weight and strength-to-weight ratios, braided composites are attractive materials for aerospace and automotive components as well as sports protective equipment (Ayranci and Carey 2008). The application of residual strength for fracture is based on the fact that, when the number of loading cycle is zero, the residual strength of the material is equal to the static strength, while at failure (n = N), it is equal to the maximum applied stress (Post et al., 2008). Using GMC, (Liu et al. 2011) built a framework for a three-scale analysis of tri-axially braided composites, and effective properties of the RUC at each scale were determined. Both two-dimensional (2D) and three-dimensional (3D) braided architectures can be fabricated in many ways, such as two-step or four-step method of rectangular braiding, tri-axial braiding, circular braiding, and other displacement braiding techniques (Bilisik 2012). a number of research teams implemented FE analysis of braided textile composites based on meso-scale geometry models. In these attempts, a RUC was used to evaluate mechanical behaviour of the whole composite structures equivalently (Pankow et al. 2012; Cousigné et al. 2013; Wan et al. 2015). J.

Montesan et al [7] conducted fatigue analysis and prediction of fatigue damage behavior of a braided type composite plate having centre hole and the fatigue analysis has been carried out using FEA software ANSYS. Fiber reinforced composites are extensively used in every sector ranging from aerospace to medical instruments due to their excellent properties such as high strength to weight ratio and high stiffness to weight ratio. Despite its crucial benefits over the conventional materials, composites are yet to be a primary choice for all high strength applications due to the complex failure mechanisms under different loading conditions because of their anisotropic characteristics (Jefferson Andrew et al., 2016). S. Anand Kumar et al. [2016] described the details study about the fracture toughness and the fatigue behaviour of spider silk and s-glass epoxy composite materials which has used in the manufacturing of modern aircraft structure using finite element method (FEM) approaches. The performance of composite materials varies under different loading conditions due to their heterogeneous nature and adverse failure mechanisms. The results of many intense researches about the strain rate effect on GFRP composites show the tensile strength and strain as less sensitive to the strain rate (Naresh et al., 2016; Naresh et al., 2017)] focussed on a review of the state-of-

the-art progressive damage analysis of braided composites with finite-element simulation. This review highlighted the importance advantages & limitations of as-applied failure criteria & damage evolution laws for yarns & composite unit cells. Ganesan et al [2018] proposed a two-parameter residual strength & fatigue life model by accounting the effects of stress ratio when the structure undergoes continuous loading. The lowest tensile strength resulting from strain rate studies has been used ultimately for conducting fatigue life & residual strength tests.

Modelling and Numerical Analysis

Damage Model Formulation

The undamaged triaxially braided PMC material is considered to behave as an orthotropic linearly elastic material, and the diffuse damage is assumed to be evolving incrementally. Damage is also assumed to be orthotropic. Since in-plane tensile loading is considered, the braided composite is subjected to a plane stress state. According to CDM theory, three internal variables representing damage are incorporated to degrade the material elastic constants for the plane stress condition. The stiffness degradation expressions are given as:

$$E_{11} = E_{11}^{0}\,(1 - D_{11})$$
$$E_{22} = E_{22}^{0}\,(1 - D_{22})$$
$$G_{12} = G_{12}^{0}\,(1 - D_{12}) \quad \text{..... (1)}$$

Where $E11$ and $E22$ are the Young's modulii, $G12$ is the in-plane shear modulus, and Dij are the corresponding internal damage variables. The superscript ''o'' refers to the undamaged material parameter. The thermodynamic potential or free energy (ρ^{ψ}) is defined for a damaged orthotropic material in a plane stress state by the polynomial:

$$\rho^{\psi} = \frac{1}{2}\left(\frac{E_{11}^{0}(1-D_{11})}{1-\nu_{12}\nu_{21}}\right)\varepsilon_{11}^{2} + \frac{1}{2}\left(\frac{E_{22}^{0}(1-D_{22})}{1-\nu_{12}\nu_{21}}\right)E_{22}^{2} + \frac{1}{2}G_{12}^{0}(1-D_{12})\gamma_{12}^{2} + \frac{\nu_{12}E_{22}^{0}(1-D_{22})}{1-\nu_{12}\nu_{21}}\varepsilon_{11}\varepsilon_{22} \quad \text{.....(2)}$$

Where ν_{12} and ν_{21} are the major and minor Poisson ratios, respectively, ε_{11} and ε_{22} are components of the strain tensor, and γ_{12} is the engineering shear strain. It is assumed in this study that the damage terms D_{11} and D_{22} are only effective when the corresponding strains are positive, i.e., E_{11} and E_{22} are not affected during compressive loading states where the effects of damage are not influential on damage evolution. From the thermodynamic potential of the damaged material, the resulting stiffness tensor is defined as:

$$c_{ij} = \begin{bmatrix} \frac{E_{11}^{0}(1-D_{11})}{(1-\nu_{12}\nu_{21})} & \frac{\nu_{12}E_{22}^{0}(1-D_{22})}{(1-\nu_{12}\nu_{21})} & 0 \\ & \frac{E_{22}^{0}(1-D_{22})}{(1-\nu_{12}\nu_{21})} & \\ sym & & G_{12}^{0}(1-D_{12}) \end{bmatrix} \quad \text{.....(3)}$$

Modelling and analysis

Finite Element Analysis (FEA) is being generally used by worldwide Engineers. Where ANSYS software has been used to analyzed the Finite Element Analysis. In this present work the FE software (ANSYS 19) is used to analyze the fatigue damage evaluations. In this present work the structure or the geometry has been taken as a braided type composite plate having a center hole includes four holes on each corner. For the analysis of fatigue damage development the modeling or the geometry has been taken as one quadrant of the total geometry because of symmetry condition. The model or the geometry has given in fig. 1. Where the plate width and height is 50mm, thickness is 25mm, radios of the centre hole and corner hole is 20mm and 8mm respectively.

RESULTS AND DISCUSSION

In the present study of prediction fatigue damage development of carbon fibre polymer matrix composite plate in order to demonstrate the fatigue damage the undamaged material properties has been given in the table 1, The model has been discredited into 21989 numbers of nodes where as the 4626 numbers of elements are used to analysis and simulate the results. & its model/geometry after mashing has been shown in Fig. 2.

For analysis of the fatigue damage a cyclic load of 55 Mpa is applied in the direction of y-axis or in the tensile direction. Fig 3 represents the loading applied on the composite plate. Where a and b are the fixed load applied where c represents the tensile load applied in y direction on the model. After simulation fig. 4 represents all the results of fatigue damages at different loading cycles such as (a) 500, (b) 1000, (c) 2400, (d) 5000 cycles.

CONCLUSION

The composite materials have resulted a greater achievement in various fields of work. now a day. This paper represents a review of the major fatigue models and time prediction methodologies for fibre-reinforced polymer composites, subjected to fatigue loadings. Here a braided composite plate is modelled having a centre hole and four holes on each corner of the plate. For conducting this fatigue damage analysis validation and comparison is done with available literature, which shows good agreement.

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Table.1. material properties of Boron epoxy composite materials

Density (ϱ)	1967 Kg/ m^3
Elasticity modulus in x plane (E_{11})	211 Gpa
Elasticity modulus in y & z plane (E_{22}= E_{33})	24.1 Gpa
Shear modulus (G)	6.9 Gpa
Poisson's ratio (ν)	0.36

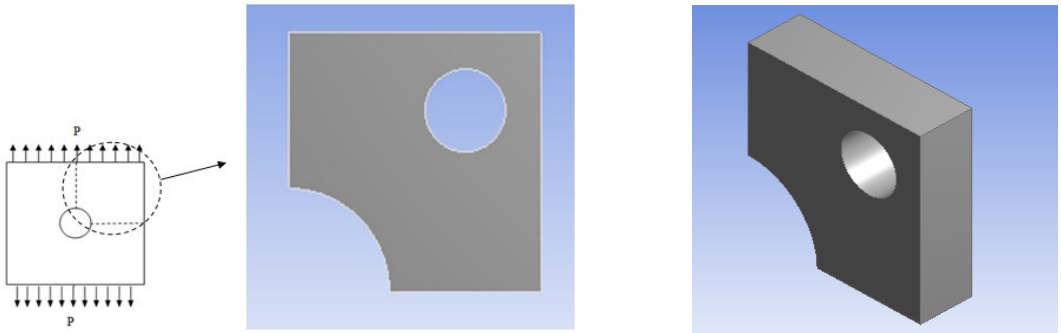

Fig. 1. Geometry/ Model of braided type composite plate

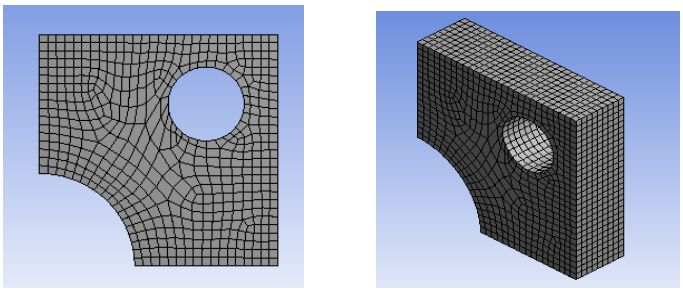

Fig. 2. geometry/model after meshing

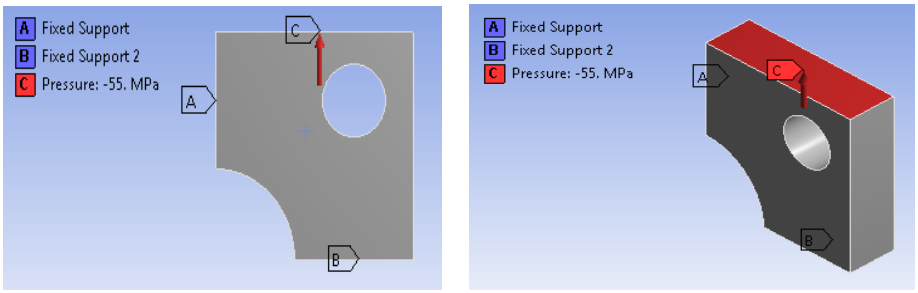

Fig.3. loadings applied on the geometry/model

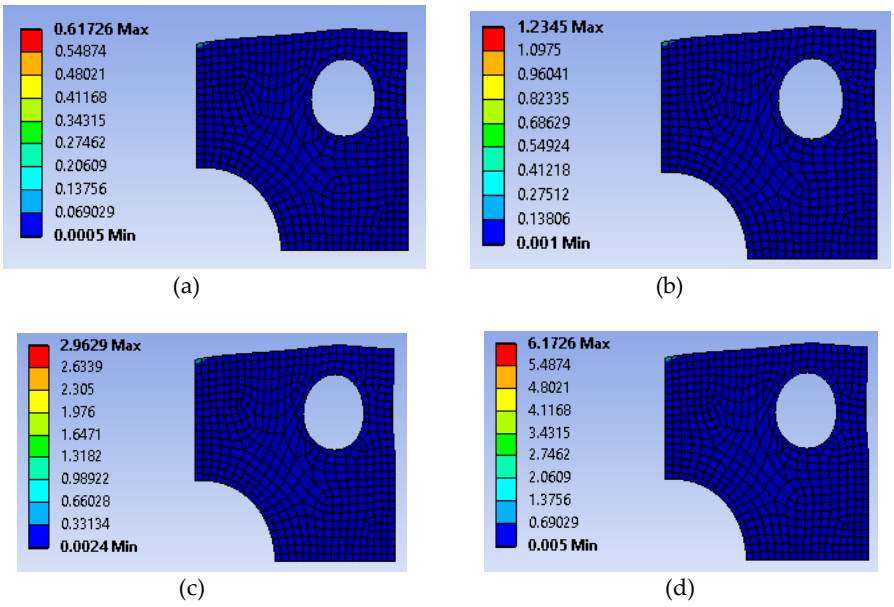

Fig. 4. contour plot of fatigue damage at loading cycle at (a) 500, (b) 1000, (c) 2400, (d) 5000

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REVIEW ARTICLE

Use of Hydrogen in Polymer Electrolyte Membrane Fuel Cells: An Overview

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ABSTRACT

Conventional fossil fuels, currently the main source of world's energy demand, are limited due to which the world will face energy crisis sooner or later. During the last few years, a good amount of research is being carried out on unconventional hydrogen fuel cell technologies to meet energy crisis, to mitigate environmental concerns about global warming and to decrease the emissions of carbon dioxide (CO_2). Hydrogen can be used in Polymer Electrolyte Membrane (PEM) fuel cells, providing a greater efficiency and producing no greenhouse gas emissions when combusted with oxygen. The only significant emission, in the process is water vapor. As Hydrogen is not a natural source of energy, it can be produced from a variety of sources making its production costlier than petroleum products. But, its excellent fuel characteristics in hydrogen fueled engines have become one of the most important research directions. This paper discusses hydrogen fuel cell technologies as one of the potential solutions to above issues and estimates the latest developments on use of hydrogen as an engine fuel. It presents possible future of hydrogen energy for better environment.

Keywords: Hydrogen energy, unconventional fuel cell technologies, PEM fuel cells, emissions, performance, production cost.

INTRODUCTION

With the growing concern for depletion of conventional fossil fuel and global warming, researchers are being interested in cleaner and more efficient automobile engines, powered by bio-fuels, electricity, solar energy and in this case, Hydrogen. Fuel cell is considered as an efficient mechanism for generation of power, because the efficiency of conversion of fuel is higher in fuel cell. The lower thermal and acoustic emission, which is generated by reaction of fuel with air is also a considerable characteristics which can be noticed in fuel cell. Fuel cells have advantages like

ease in operation, maintenance, mobility and flexibility in size also. Thus, they present a potential source to be used in places where clean electric power and conventional internal combustion engines work reliably. Typical Hydrogen fuel cell thermal efficiency ranges from 40 to 60%, which is considerably more than IC engines (20 to 30%) [1, 2]. At partial load, efficiency of Hydrogen PEM fuel cell systems is more than full load and hence most suitable for the use in engines operated at partial load, e.g. when driving in city roads. Also it cells produces zero CO_2 emission due to H_2 fuel. Transportation noise in cities is also less by use of the cells. Fuel cell automotive can be applied as generators of electricity when parked at houses and offices. From this perspective, the use of PEM fuel cells is suitable, not only for personal vehicles, but also for public transports like buses [3]. PEM fuel cell automotive have less no. of hydraulic and mechanical subsystems, in comparison to conventional engines, give better flexibility in design, less platforms and so more efficient production procedures can be developed, which leads to cost cutting. The cost cutting potential of PEM fuel cells should be considered and in accordance with the alternate vehicle in future auto-market [4].

II. PRINCIPLES OF POLYMER ELECTROLYTE MEMBRANE (PEM) FUEL CELLS

PEM cells, also known as Proton Exchange Membrane fuel cells, give high level of power density and offer advantages of low volume and weight compared to regular fuel cells. These fuel cells only require hydrogen, oxygen and water to operate. Storage tanks or reformers supply pure hydrogen in these fuel cells. Solid polymer is treated as electrolyte and porous carbon plates are treated as electrodes in PEM fuel cells. The fuel cell also contains platinum (Pt) catalyst [5, 6].

PEM fuel cells operate at lower temperatures than regular fuel cells. The typical temperature of operation is around 80°C [7]. Operation at the low temperature allows them to start quickly requiring less warm-up time and eventually results in less wear of the system components and better durability [8]. But, the fuel cell needs a metal catalyst, preferably Platinum (Pt), to separate protons and electrons of hydrogen. This adds to cost of the fuel cell. The Pt catalyst is sensitive to poisoning by Carbon monoxide (CO), which makes it requisite to apply another reactor, which reduces CO in fuel gas. This additional reactor also adds to the cost [9]. Hydrogen is produced by means of a reforming reaction carried out either externally or internally. In a fuel cell operated at high temperatures (e.g. molten carbonate fuel cell), the heat is used for generating H_2 and CO_2 as well as facilitating electrode reaction simultaneously [10]. In a low temperature fuel cell, the reforming process occurs in an external reformer and the hydrogen produced is consumed to generate electricity. Figure 2 shows main components of fuel cell system.

If natural gas has to be used, it is processed in a reformer to create hydrogen rich fuel. Figure shows schematic diagram of H_2 and O_2 fuel cell [11]. The processed fuel is fed to the fuel cell between the end plate (bipolar separator plate) and the nickel anode. Simultaneously, air (oxygen) is cleaned with filters and then channeled between the cathode and bipolar separator plate (end plate). Sandwiched in between the anode and the cathode is the electrolyte (40% KOH) [12, 13]. This porous material enables the hydrogen and oxygen to chemically react. Electrode reactions occur releasing free electrons that flow an external circuit through load and to the cathode. The following reactions take place in the fuel cell:

Anode: $2H_2 + 4OH^- \rightarrow 4H_2O + 4e^-$
Cathode: $O_2 + 2H_2O + 4e^- \rightarrow 4OH^-$
Cell reaction: $2H_2 + O_2 \rightarrow 2H_2O$

Mechanism of PEM cell is very basic. Hydrogen fuel cell was first demonstrated by scientist William Grove in 1839, which is given in Figs. 1 and 2. In Fig. 1, the water electrolysis producing oxygen and hydrogen by passing the electric current is shown [14]. However, in Fig. 2, the H_2 and O_2 are recombined, and the electric current is being produced. The figures demonstrate the basic principle of PEM cell [15, 16].
In the first step, hydrogen is combusted in the simple reaction to obtain water (H_2O).
The current produced, in the experiment, is less, which is because of:

- The area of contact between the electrolyte, gas and the electrode is small.
- The distance between two electrodes is large and so the electric current is resisted by the electrolyte. To address this, the electrodes are manufactured with plane surface with a coating electrolyte as shown in Fig. 2.

Each electrode has pores which allow the penetration of the gas and electrolytes from the both sides. It gives possibly the maximum contact of electrolyte, electrode and the gas. But, to show the reaction of H2 and O2 which gives the production of electric current, and place from which electrons are obtained from, separate reactions should be considered which occur at the electrode [17]. It varies with the change in types of fuel cells. At the anode, the H2 ionizes, which creates H+ ions because it releases electrons.

$$2\,H2 \rightarrow 4H^{++} + 4e^{-} \quad (2)$$

Energy is released in the reaction. At the cathode, O2 reacts with electrons released at anode, and H+ ions which forms H2O.

$$O2 + 4e^{-} + 4H^{+} \rightarrow 2H2O \quad (3)$$

The two reactions need to be continuous for which, the cathode should be continuously provided with electrons from anode [18, 19]. H+ ions or protons should pass the electrolyte also. The acid is liquid with free H+ ions, and so it fulfils the requirement. It can be seen from Eqns. 2 and 3 that two H2 molecules are required for one O2 molecule when the fuel cell is at balance. Also the electrolyte should allow H+ ions, not electrons, to pass it [20] or electrons can go by inside of the electrolyte, not in the circuit external to it. In the second case, the alkaline electrolyte cell, the basic reactions are same, but the reaction at each electrode is separate from the other. In alkaline electrolyte cell, hydroxyl (OH−) ions move and at anode, react with H2, which releases energy and electrons, and produces H2O also [21].

$$2H2 + 4OH^{-} \rightarrow 4H2O + 4e^{-} \quad (4)$$

At cathode, oxygen does reaction with electrons from the electrode and water from electrolyte, which forms OH− ions.

$$O2 + 4e^{-} + 2H2O \rightarrow 4OH^{-} \quad (5)$$

The reactions should be continuous, for that, OH− ions should pass the electrolyte and the circuit should be formed for the electrons to travel from anode to cathode [22]. Also comparing Eqns. 4 and 5, twice hydrogen is needed as oxygen with the acid electrolyte. Though consumption of water occurs at cathode, it is reformed at anode in double speed [23, 24]. To use PEM cell effectively, huge engineering mechanisms are needed to be applied in system. When being supplied at a load, the external properties of PEM fuel cell should match the requirement of load. When PEM cell is being supplied at a load, which varies, is it even more challenging [25]. For the most of the cases, an interface is required, between the PEM cell and the load, which can be a power electronic converter. For the performance to be dynamic, various operational variables, like temperature and injection rate of fuel, are required to be controlled. So a mathematical model is needed for design and performance control [26, 27]. Essential steps for fueling of H2 are [28]:

- First the station of fueling should be supplied with H2. H2 can also be produced inside the tank, but for this case, fueling stations are being considered. The hydrogen fuel can be delivered to the station by truck, train and pipeline.
- Storage of H2 can be in form of liquid or gas at the fueling station.
- As the state of hydrogen stored, can be in separate form the form which is needed at the time of fueling, the fuel state conversion from liquid to gas for final supply, is required.
- H2 is fueled to vehicle tanks.

For the case, where hydrogen can be produced onsite, it can be obtained from electrolysis of H2O. In the case, if engine is on load, the water is obtained from storage and passes inside PEM cell, where the H2 is produced and used as fuel. H2 is not stored as a gas, when engine is not on load that is when the engine is off, only water is kept in storage which if safe for passengers [29, 30]. But the method is not economical and not discussed in the current paper.

III. SUBSYSTEMS OF PEM FUEL CELLS

PEM cell automobiles have an electric drive train to generate electricity electrochemically, from fuel cell. Along with that, other subsystems of PEM cells are [31]:

A. H_2 storage and fueling subsystem
B. H_2 delivery subsystem
C. Electric drive subsystem
D. Power management and electric propulsion subsystem

Along with these subsystems, some fuel cell vehicles are attached with more mechanisms to increase the efficiency of PEM cell, like equipment to save the energy dissipated during braking. Figure 3 shows each of the subsystems and locations of them, within a H2 vehicle drive train [32]. The paper focuses on the H2 fueling and fuel storage, fuel delivery, electric drive and fuel cell power management subsystem.

A) Hydrogen Storage and Fueling Subsystem

The common form to store and supply H2 on board, is the form of compressed gas. In vehicles of current development, the typical storage pressure of H2 is 35 M Pa. Compressed- hydrogen systems operating at pressure of 70 M Pa are being developed also [33, 34]. H2 is transported from storage system to stack of PEM cells, in a subsystem called pressure piping, going by 2 to 3 stages, which decrease the pressure of H2 to 0.034 MPa, at the time when it enters the stack of PEM cells [35]. Primary element in the subsystem is compressed- H2 fuel tanks. As H2 has a low energy density per unit volume, the design of fuel tank should be proper for supplying required amount of H2 to be within practical driving range [36]. To address the limitations, fuel storage subunit is designed to take very little space and composite materials with low weight are used to produce the subunit [37, 38]. Also, to address the low energy density, the storage tank is designed to store H2 at high pressure [39].

B) Hydrogen Delivery Subsystem

Delivery of H2 from fuel tank to the stack of PEM cells is by a series of piping, flow meters, filters and pressure regulators, which is considered as the H2 delivery subsystem. Primary requirement of H2 flow control system is efficient delivery of H2 to stack of PEM cells, at stable temperature and pressure for PEM cell operation at full range operating condition [40]. Delivery of H2 should be at a specific rate, even when the pressure in storage tank drops or any change occurs in ambient temperature. The specifications for delivery of H2 are decided by storage pressure in initial condition and the pressure at duty cycle [41, 42]. Materials of piping system should be selected and then tested in such a way that it should be able to maintain the pressure without rupture [43].

C) Electric Drive Subsystem

Along with providing the electricity required to operate the drive motor, electric drive system produces electricity for charging vehicle batteries and capacitors. The PEM cell contains a stack of hundreds of fuel cells in which H2 and O2 electrochemically react to produce the required electricity [44] and they can continuously produce it when delivered with pure H2 and O2, simultaneously [45].

D) Power Management and Electric Propulsion Subsystem

PEM cell vehicles are powered with electric motors, which are capable of producing and supplying mechanical energy to drive axle, by conversion of electrical energy produced in the cell. Batteries and ultra-capacitors are the other components of the subsystem [46]. Most of the PEM cell vehicles have front-wheel drive, with electric drive motor and drive train mounted in the engine compartment, transverse along front axle. The pattern is similar to traditional internal combustion vehicles. For large SUV-type vehicles, all-wheel drive is provided with 2 electric motors, one along front axle and one along rear axle, and 4 compact motors are provided, as one for every wheel.

IV. ADVANTAGES AND DISADVANTAGES OF PEM FUEL CELLS

For the design, investment and applications of the fuel cells, the advantages and the disadvantages of fuel cells need to be considered. The main advantages of the fuel cells are: The PEM fuel cells are more efficient than regular fuel cells, simple to design and manufacture and flexible for wide application range. Also the PEM fuel cells create low emissions and are economy and environment friendly. These fuel cells are more silent in operation also [47]. The main disadvantages are: The cost of the hydrogen infrastructure, production and refueling of Hydrogen and Platinum catalyst. The high cost of construction and storage can be compensated by application of fuel cell in public transport vehicles. Construction of a water infrastructure should be in accordance with cost effectiveness for less maintenance requirement [48].

CONCLUSION

Applications of PEM cells in automobile sector will be successful when manufacturing and pricing of these vehicles will be rigorous and hand in hand with internal combustion engine vehicles. Design and testing of PEM cells should be analyzed with finite element methods to prove efficiency of the parts and metals used in production of them. PEM cells are most suitable for applications in mobile powers as their power density is high and temperature of operation is low. Still all the applications of PEM fuel cells are as fuel cells in hybrid vehicles. The hybrid combination results in the better response and ability to obtain the best characteristics of both PEM cell and conventional batteries. PEM cells can actively decrease air pollution, when a large population will start using the technology. In twenty first century, H2 fuel can be part of national economy of any country and PEM cells can be used to generate a large amount of electricity for transportation sector. So we should shape up PEM cell not as a dream but as a good solution to address the demand of energy and environment of the future.

V. FUTURE SCOPE

Fuel cells using hydrogen will have a major role in automobile and transportation industry in the coming days. Enough investigation is required to produce fuel cells in large amount at reduced price in order to make it commercialized. It could be hoped that transportation, power plants and electricity generators used with fuel cells will be a better alternative in the coming days.

Conflict of Interest

The authors declare no conflict of interest.

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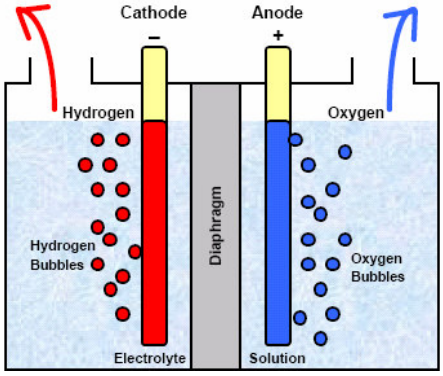

Fig. 1 Standard electrolysis [14]

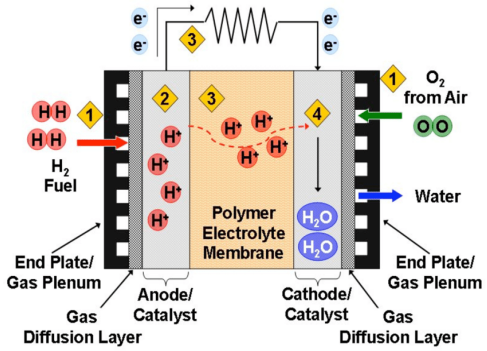

Fig. 2 PEM electrolysis [15, 16]

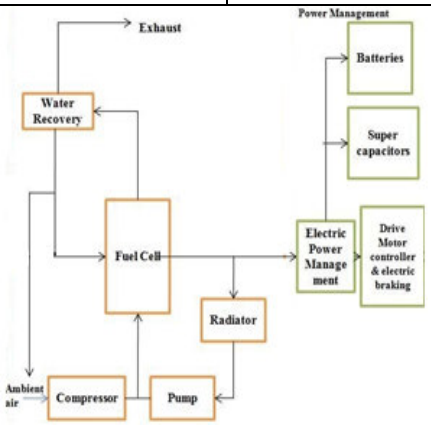

Fig. 3 Subsystems of PEM fuel cell [32]

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RESEARCH ARTICLE

Assessment of Applicants' Response on the Implementation of RTI Act: A Case Study of Srikakulam District

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ABSTRACT

Right to Information or the Freedom of Information has the ability to generate more controversy and heated debate than virtually any other aspect of contemporary government and administration. Having experienced certain important contents of RTI act from different literature and experiences, researchers of this study focus on the challenges faced by the applicants since the legal systems, administration, policy and practices of RTI is unclear in terms of implementing practically. Hence the aim of the study is to evaluate the influence of the challenges on the implementation of RTI in Srikakulam District. This study carried out through a method mix of both descriptive and exploratory research with qualitative and quantitative approach. The respondents were selected through convenience sampling from Srikakulam district determine to the size of 388 all the selected variable of challenge have been analysed with comparing means and ANOVA to know the impact on the successful implementation of RTI through positive public response. It is found through interpretation that almost all the challenges are significant enough and influence a lot on implementation errors of RTI. A couple of suggestions with respect to the awareness, PIO attitude and other variables have been offered for the maximum possible utilization of RTI with the least errors.

Keywords: RTI, Challenges of implementation, public response, Srikakulam

INTRODUCTION

Freedom of expression as a key role, the system through Right to Information act process the democratic ruling by governments as coded in Article 19(1) (A) of the constitution being called as a pioneer for the liberty majorly and thereby protects other aligned activities to be participated by the public with freedom. Acquisition and dissemination through the same article is entitled to process without any hindrance which leads to form an accomplished opinion by any applicant.

If any individual fails to get the information or pay against getting information or else feel sensitive or worthless to pay because of public apathy. It tends to be stated as the same individual has no freedom. It has been a continuous experience by the public that the departments concerning transactions and communications of financial markets to government, from national security to education, form multinational corporations to small employers, from police to social welfare, medical treatment and social services have shown a contempt kind of results in implementation since they fail regularly in storing and disseminating the information to the public who need it for several liberty reasons. Information being taken to light and being transparent enough would pave the way for the eradication of corruption which in turn help the public with respect to the information comfort and trustworthy the confidence to be created in public with respect to the information given whenever needed without any flaws would in turn be a dexterous consequence of initiation to eradicate corruption. This is possible with the moment of implementing RTI properly since the legal rights are attributed with the transparency is evitable and accountability is assured. it also increases the citizens 'participation in governance and the quality of life of citizens would thereby be enhanced with integrity and rights' fulfilment.

RTI ensures the right more enforceable to question, examine, audit, review and assess government acts and decisions which should be are trusty with the principles of public interest, correctness and justice. The access to public is expected to improve from the right would rather get modified with certain constructive conditions to curb and convert to effective usage. On the other hand , it should also be noted that the concept is not completely existed in our constitution, at the same time, employing RTI is indifferent in many countries in line with its establishment (H.M. Seervai, 1976). In India, Supreme Court has had several decisions to develop the legal stand of RTI time to time.

There have been several positive and negative experiences from the applicants where in some organisations provide accurate information in time but, most of the other organisations do not. The reason behind this are vary enough and turns into the challenges could not be well absorbed by the public. The process from receiving the application to responding positively has innumerable challenges amalgamated with severe gaps. The researchers with the substance acquired from pilot study, tried to expose the implementation hurdles of the applicants where the purpose of RTI is not well served. Having studied certain important contents of RTI act from different literature and experiences, researchers of this study focus on the challenges faced by the applicants since the legal systems, administration, policy and practices of RTI is unclear in terms of implementing practically. There have been real time experiences at different government offices and the previous research experiences had been taken into consideration and analysed to measure the severity of the challenges faced by the public. Public response in this issue has been finalised with intensity.

Objectives

The objectives of the study is to

- Study the Implementation process of Right to Information act in India
- Identify the challenges to access the right to information access by public.
- Assess the public response towards implementing the right to information act in Srikakulam District
- To evaluate the influence of the challenges on the implementation of RTI in Srikakulam District

RESEARCH METHODOLOGY

The study was carried out with a cross-sectional design survey research to achieve the stated objective. This research is both explanatory and descriptive where in researchers have preferred quantitative and quantitative approaches for achieving the purpose of the study. The target population consisted of the public from Srikakulam district (A.P.) who pursued information from government offices through RTI act with respect to the proportion of rural and urban people irrespective of demographical preferences. Considering the purposes of this study, primary and secondary data collection methods have been carried out. In view of the information needed for the study, and the nature of the target population,the selection of respondents was proceeded by using Non-probability with convenience sampling technique to select the respondents from the study area.

The self-administered questionnaire contained the major independent variables in order to comprehend the challenges faced by the public in implementing the act of Right to Information. The measures were developed based on literature and empirical studies conducted previously. The questionnaire included closed ended questions of Likert scale type.

Related Literature

There have been enough literature and documents related to RTI act which can be discussed as the fundamental dicta, but the purpose of the study needs to discuss the literature related with the challenges or problems that the public who apply for the information to RTI and the severity or the intensity of the problem which prevent from the successful implementation of RTI in not only Urban but also Rural places. Undergoing the study of RAAG and PWC, the established challenges epitomised are as follows.

- Increasing level of awareness for certain communities are found highly needed since proper enlightening drive organized by the government in India is yet to be accomplished.
- Quality of RTI awareness in common public is to be emphasised, particularly among women, rural people and OBC/SC/ST category public which is found very low.
- Availability of user guidelines for RTI is another issue being considered as a challenging factor, whereas, with reference to Section 26 of the RTI Act, the responsible Government is indebted to print and dispense user guides for the people that seek information.
- The standard form of RTI assists in receiving straightforward information such as personal details and other requirements which accommodates Public Authority to classify the nature of information requisitions so that it can be established as a suo-moto disclosure.
- There have been many inconvenient hurdles while submitting RTI application where the channel noise confuses the public with the prescribed language, media, technology and payment.
- Submission of fees for application is to be made convenient since the confusions exist with cash and demand drafts, which troubles the citizens.
- Under Section 5(3) of RTI Act, PIO has to support citizens in filling in RTI applications. But there is a high dissatisfaction for the same is not served in reality.
- Limitations confronted in inspection of records are numerous since some applicants require PIOs to collect and analyse the data for previous years. However, it is noted that PIOs never do it and advised that they should obtain the same.
- It is highly observed that the information required by the applicant are not able to get in time so as considered as a big failure to provide information within prescribed time period of 30 days.
- Another problem of appeal process is very lengthy and the authority is not given judicial power regarding this.

- There is an ambiguity whether the higher judiciary of the country is covered under the provisions of the RTI Act or not. Unless the higher judiciary starts considering its responsibility, complete transparency is impossible.

The present study has included four influencing challenges from the above specified challenges i.e. Low level of awareness, Non-availability of user guides for RTI implementation for information seekers, Constraints faced in inspection of records, and Failure to provide information within 30 days which have been found important at the present situations in Srikakulam district. Researchers also conducted a pilot study with experts and administrators from which other variables such as PIO willingness/Attitude to provide information, Responsiveness from state information commission and Applications with political interest rather than public interest have also been included.

Analysis And Interpretation

Challenges faced by the public from the implementation of RTI today: It is found and easily understood that the problems faced by the public while implementing RTI in the district of Srikakulam have been severe enough as the comparing mean values of all explored in table 1. However, the element "Responsiveness from state information commission is poor" carries the highest mean value of 4.0917 and the element "Applications are with political interest rather than public interest" shows the least mean score with 3.1101. Hence, it can be understood that the severe problems while applying or implementing RTI in Srikakulam district are poor response from state Information commission, Negative attitude of PIO and Availability of Low level of information for they carry 4.0917, 3.9907 and 3.9000 respectively. At the second rate the elements influencing moderately carrying mean values are around 3.7 as shown in the table are Non-availability of User Guides, Constraints faced in inspection of records and Failure to provide information within 30 days represent the intensity is moderate but the public.Quite surprisingly, the respondents have shown a little disagreement towards a blame that the applicants are seeking information from the government offices through RTI out of political interest rather than public interest.

Table 2 shows the relationship among the severity of different challenges and the successful implementation of RTI act. The F values between dependant variable and independent variable starting from "Non-availability of User Guides" is 108.080, "Constraints faced in inspection" is 67.320, "Failure to provide information within 30 days" is 92.474, "PIO willingness/Attitude" is 234.606, "Responsiveness from state information commission" is 88.194, "Low level of information" is 66.405 and "Applications are with political interest rather than public interest" is 112.449. The values for all independent variables show high significance with 0.000 at the level of 0.01. So it can be concluded that all the factors are showing high significance on the Implementation of RTI in Srikakulam district. Hence it can be interpreted that the variables selected by the researchers have been proven imperative and have high level of impact and influence.

CONCLUSIONS

The utmost dissatisfaction has been shown by the respondents towards the administration of government offices handling RTI act and delivering services in line with all the variables/ problems which are considerably significant.
It can be concluded that the poor responses from state Information commission, Negative attitude of PIO and Availability of Low level of information are considered as the most painful for the respondents at the first rate. On the other hand, the elements influencing moderate are Non-availability of user guides, Constraints faced in inspection of records and Failure to provide information within 30 days represent the intensity is moderate but the public.

RECOMMENDATIONS

1. Since the problems are all significant enough, the execution of RTI act is yet to be flexible with respect to the applicants' awareness and the government should incorporate certain amendments in the act to make it deliverable at ease.
2. PIO's responsiveness being negative is not to be excused at all. PIO's attitude provide information with accuracy as per norms should be made mandatory.
3. Achieving the objectives of RTI act with transparency as the main goal should not lead to any corruption and the related authorities should focus on the continuous monitoring with accountability.
4. Awareness of RTI act to the rural community is to be highly promoted since there are very less people found known about this act. Though some know about this as a basic knowledge, knowing how to implement is a big dilemma.

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Table 1 Comparing means of public response on implementation challenges

Challenges faced by the public	N	Mean	Std. Deviation
1. Non-availability of User Guides for RTI implementation for information seekers	110	3.7431	.86499
2. Constraints faced in inspection of records	110	3.7238	.95570
3. Failure to provide information within 30 days	110	3.7000	.95351
4. PIO willingness/Attitude is negative to provide information	110	3.9907	1.29946
5. Responsiveness from state information commission is poor	110	4.0917	1.05006
6. Availability of Low level of information	110	3.9000	.86682
7. Applications are with political interest rather than public interest	110	3.1101	1.11670

Source: Survey result, 2019

Table 2 ANOVA[a]: Impact of the challenges on the execution of RTI

Model	Sum of Squares	Mean Square	F	Sig.
1) Non-availability of User Guides for RTI implementation for information seekers	206.191	51.548	108.080	.000
2) Constraints faced in inspection of records	193.975	32.329	67.320	.000
3) Failure to provide information within 30 days	180.234	45.058	92.474	.000
4) PIO willingness/Attitude is negative to provide information	220.390	110.195	234.606	.000
5) Responsiveness from state information commission is poor	136.268	45.423	88.194	.000
6) Availability of Low level of information	164.595	32.919	66.405	.000
7) Applications are with political interest rather than public interest	166.889	55.630	112.449	.000

Source: Survey result, 2019

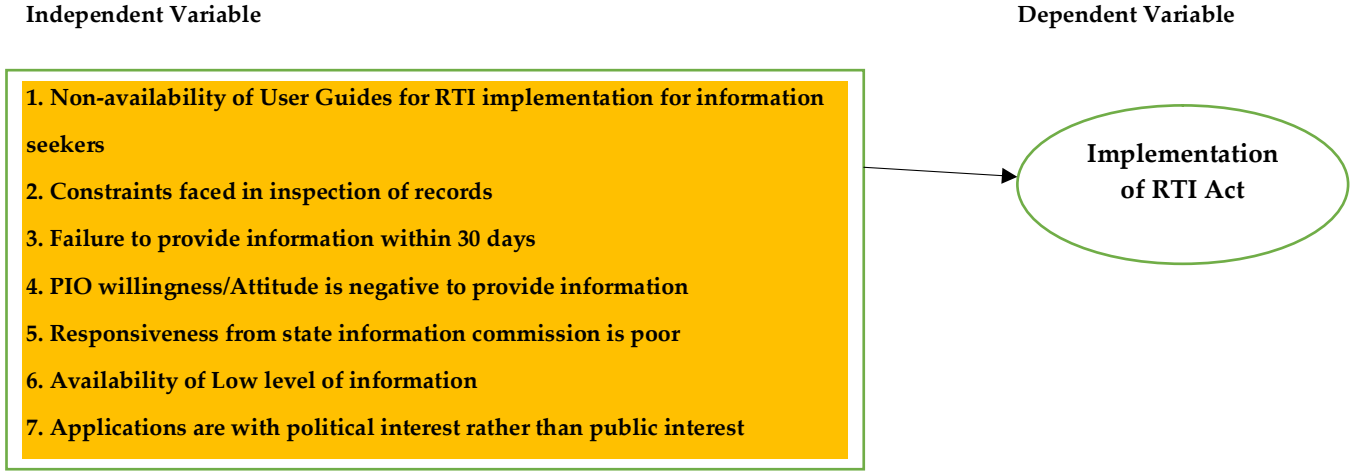

Figure:1. Conceptual Framework (Source: Modified from RAAG and PWC study)

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RESEARCH ARTICLE

Designing a Sharply Estimated Natural Solution of Acetone-Water: Ratification as Refrigerant in Vapour Compression System

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ABSTRACT

Halogenated refrigerants of present generation drops down the ozone layer and catalyses global warming. Replacement of synthetic halogenated refrigerants by natural organic substances is the front line research challenge over last few decades. The recent work is an endeavour to estimate a sharp range of Acetone-water ratio that ratifies to a suitable refrigerant in vapour compression units with pros and cons. The natural solution in designed ratio was retrofitted in a vapour compression unit coupled with engineering equation solver (EES) considering trendy R-134a as base line refrigerant. The ratifying parametric conditions were calculated in terms of $(COP)_{ref}$, nontoxic character ,reasonable compression ratio, work input, flammability, durability, stability & environment friendliness. In comparison to synthetic refrigerant R-134a the designed ratio of Acetone-water solution was echo friendly with proximal $(COP)_{ref.}$ The designed ratio was non corrosive with greater thermal and chemical stability for domestic refrigeration and air conditioning units.

Keywords— Vapour Compression Refrigeration System, Acetone & Water Solution, designed ratio, process development, validation.

INTRODUCTION

Recycling the refrigerant by change of phase through vapour compression system is the evolutionary technology of recent generation. The technology has been widely adopted in refrigerating, air conditioning, heat pumps and water chillers unit. The context of technological evolution of refrigerants includes hydrocarbons (HC), hydroflurocarbons (HFC), HFC/HC, hydrochloroflurocarbons, (HCFC), carbon dioxide (R744) and ammonia (R717). Amongst these working fluids halogenated refrigerants are rampantly used in vapour compression systems reasoning its good thermodynamic and thermo-physical properties. However the toxic nature of these fluids vitiates the ozone

depletion potential (ODP) and global warming potential (GWP). International refrigerant protocol standard (Montreal and Kyoto) refrains use of halogenated refrigerants in the vapour compression systems. However it does not encompass hydrochloroflurocarbons (HCFC) till 2040, in developing countries like India outgrown by 2030 [1]. Use of HCFC as refrigerant recently drops down in developed nations. Minimizing the emission of six categories of green house gas contributed by hydroflurocarbon (HFCs) refrigerants has been mandated by United Nations Framework Convention on Climate Change (UNFCCC) [2]. In recent context designing right combination of echo-friendly mixture finds new way of investigation. Combination of HC and HFC mixtures reduces GWP. However the combined mixture is instantly inflammable that restrains its use in bigger capacity units [3]. Smaller units prefer HC refrigerant mixtures for domestic purpose that requires lower volume of refrigerants.

HFC mixtures are ozone-friendly associated with significant GWP and immiscible to mineral oil, which require synthetic lubricants (such as polyolester). The presence of synthetic stuffs in HFC are hygroscopic in nature, expensive, causes itching in contact with skin and provides way to several service problems in overhauling [4]. Problems associated with HC and HFC refrigerant mixtures are overcome by blending hydrocarbons with HFC that facilitates miscibility (with mineral oil) and reduces flammability [5]. Basing on investigations HFC/HC mixtures are miscible with mineral oil with one-third GWP than HFC, when used alone. Hence HFC/HC mixtures can replace halogenated refrigerants [6].Use of natural working fluids as refrigerants have been reported in VCR and VAS [7].Use of different pure HC refrigerants have been reportedly experimented [8].Evolutionary development of pure refrigerants from early use to the present has been reported [9]. Investigations on environment-friendly alternatives reported that refrigerant mixtures are the replacement for halogenated refrigerants [10].

In recent context no specific or very little investigations have been reported on refrigerant mixtures. Hence, the present work more broadly investigates the performance of new refrigerant mixture: Acetone water with special focus on its possibility as an environmental friendly refrigerant. Moreover, the study involves estimation of echo friendly impact, economy of use in fraternity with retrofitting, forecasting of refrigerant properties in the scenario of refrigeration and air-conditioning segment with technical pros and cons.

MATERIALS AND METHODS

Selection of materials

The UNFCC mandates phases-out pure halogenated refrigerants. A very narrow range of pure fluids exists in nature that exhibits parallel properties to halogenated refrigerants. Hence mixture of two or more refrigerants that shows adjustment of properties and behaves as a single substance is desirable. Azeotropic mixtures evaporate and condense as a single substance with their properties being different from those of constituents. Boiling point of azeotropes is lower than either of their constituents used as refrigerants. Acetone water solution was azeotropic in operating range of temperature and pressure. However further increase in temperature and pressure made it nearly azeotropic mixture. Nearly azeotropic mixtures are having very low temperature glide in the range between 0.2 and 0.61^0 C that does not affect the hardware design. So in present investigation azeotropic mixture of Acetone to water in the ratio ranging from 54: 1 to 76:1was trialed. The range of ratio was designed basing on unwieldy iterative trial and error with evaluation of properties.

Material characterization

Acetone commercially known as propanone, is an organic compound with the formula $(CH_3)_2CO$. It is the simplest and smallest ketone, colourless, volatile, flammable liquid with a characteristic odour. Acetone is miscible with water. Acetone is produced and disposed of in the human body through normal metabolic processes. The other chemical identity specifications were given in Table.1.

Process development and validation

The Acetone water refrigerant in designed ratio was retrofitted to a test rig using R-134a as baseline refrigerant. The COP of both refrigerants was recorded for comparison. The technical specifications of the test rig were: Model UPSON, Model number-URF-M5, Rated voltage 240V, Electricity consumption 0.5kWh/24h & Power 90W, and Weight 19kg, Volume 47L coupled with engineering equation solving software (EES).The major feature of EES is the high accuracy thermodynamic property database that is provided for hundreds of substances in a manner that allows it to be used with the equation solving capability. Refrigerants retrofitted alternately were R-134a and Acetone water. The flow diagram of the refrigerant test rig was depicted in Fig.1.

Rig thermodynamic processes

Process: 1-2(Compression)

The process was adiabatic. Work was done on refrigerant ($W=v.\ dp$) by energy input. Compression was dry, wet or super heated depending upon the phase of the refrigerant at that instant.

Process: 2-3(Condensation)

The process was isobaric rejection of heat from refrigerant to atmosphere.

$$Q_1=W_{C+}Q_2$$

Process: 3-4(Expansion)

The process was adiabatic retrofitted with capillary tube expansion valve.

Process: 4-5(Evaporation)

The process was isobaric heat addition from desired cooling space to the evaporator flooded with refrigerant. Figure.2 shows the flow diagram of different processes with phase change.

$$Q_2=m.c_p.dt$$

Refrigerant mixture

The research evolutionary gestation period of R134a emerged out with discovery of the damaging effect of CFCs and HCFCs refrigerants to the ozone layer. It is known as Tetrafluoroethane (CF3CH2F) of HFC refrigerant family. Present generation of refrigeration and air conditioning rampantly use it as CFCs and HCFCs replacement in centrifugal, rotary screw, scroll and reciprocating units. It is safe for normal handling as it is non-toxic, non-flammable and non-corrosive. Currently automotive sectors use it in interior air conditioning. The properties of R134a were summarized in Table.2.

However UNFCCC mandates use of HCFC till 2040, in developing countries like India outgrown by 2030 [1]. The combined mixture is instantly inflammable and raises Global warming potential (GWP) that restrains its use in bigger capacity units [3]. Hence in present context the search for an environmental friendly refrigerant was prevalent focusing on proximal COP. Acetone water mixture in designed ratio 54: 1 to 76:1was such a nearly azeotropic refrigerant on which attention of investigation was concentrated to find its possibility as an environmental friendly refrigerant. A summary of chemical properties, structure and thermo chemistry of Acetone to be used as primary component of refrigerant mixture was given in Table.3.

RESULT AND DISCUSSION

Selection of materials

Acetone was preferred as primary constituent of novel nearly azeotropic mixture refrigerant considering its ball-beam structure, dimensional structural formula & bond order configuration. The structural geometry was shown in fig.3. The structural geometry contributes to : thermal and chemical stability, low density(low pumping work to circulate), assessable range of boiling point(not achieved in halogenated refrigerants),non toxic nature, comparatively higher emissivity & refractive index than conventional refrigerant(low compressor work), low freezing point of -78^{o}c(superior cooling effect), stoechiometric pressure impact on conduit walls(latent heat transfer),better lubrication property(no scaling inside copper conduit at elevated temperature & pressure), odorous(easy leakage detection) and negligible GWP & ODP.

However its high inflammability, low density and low specific heating value were imperative issues to be addressed before considering its possibility as primary constituent of refrigerant mixture. High flammability restrains its use in bigger units, low density increases possibility of leakage in conduit and valves when compressed and low specific heating value is not tolerable. The associated problems were addressed by mixing water with Acetone to form a nearly azeotropic refrigerant solution in the ratio of 54:1 to 76:1. Mixing of water increased its density and specific heat thus decreasing chances of leakage and manages the sharp increase in temperature while adding heat. It also moderates the flammability risk. The mixing of water in designed ratio (54: 1 to 76:1) did not intervene any irregularity in nearly azeotropic behaviour of the mixture refrigerant over a wide temperature range as it was readily soluble to Acetone. So, the solution of Acetone & Water (54: 1 to 76:1) holds optimized characteristics of a refrigerant. However the designed ratio (54:1 to 76:1) was to be fairly maintained, any violation may cause serious damages to the system. Excess water causes corrosion, valve choking and seizure of piston or vanes of compressor unit. It also impairs heat absorbing & radiating nature and compressibility of refrigerant mixture causing decreased $COP_{ref.}$. Fair maintenance of designed optimal ratio (54:1 to 76:1) was the investigation objective of present research endeavour to develop a better ever refrigerant mixture. The experimental thermodynamic behaviour of the refrigerant solution was presented in table.4.

Material characterization

Choosing Acetone as primary constituent of refrigerant mixture was rationalized to its lowest contribution to global warming, considering various hydrocarbons.Table.5 represents the contribution of various possible hydrocarbon refrigerants to global warming.The other inference of identifying Acetone as primary constituent was its fairly change of phase with respect to designed range of temperature and pressure and thermodynamic behaviour as a refrigerant. The figure.3 explains the pressure and temperature oriented phase change and table.6 represents the thermodynamic behavioural comparison of Acetone with other refrigerants in critical range of pressure and temperature.

The comparative thermodynamic behaviour investigated that Acetone inferred: high latent heat of vaporization, suction gas density, no excess pressure inside evaporator and condenser, chemically stable with water, non-corrosive, non-toxic and environment friendly. The flammability was moderated with adding water in designed ratio (54:1 to 76:1). Other favorable result was critical temperature and triple points were well beyond the designed range of working.

Process development and validation

The test rig was initially charged with R-134a as baseline refrigerant. Performance of R-134a was evaluated from the parametric conditions of compression, condensation, expansion and evaporation employing engineering equation solver software (EES) coupled with test rig [11]. Secondly the rig was retrofitted with presently developed acetone

water solution refrigerant in optimal ratio 76:1 to record the software generated performance. The performances of both the refrigerant were compared considering R-134a as baseline refrigerant. Comparative results obtained were presented in Table.7.The parametric inputs were the working temperatures at superheating, sub cooling and compressor speed (Ta, T_{ff} & T_{fz}). Thus, for a given set of guessed values for P_e , P_c , h_1 and T_R , the compressor sub-model calculates h_2 , the condenser sub-model estimates h_3 and T_3=T(P_c,h_3), the internal heat exchanger sub-model calculates h_4 and T_1 , and the evaporator sub-model calculates h_5 and T_5 =T(P_e ,h_5).

CONCLUSION

The present investigation validated a nuance in COP between R-134a and Acetone water mixture. The proximal COP of Acetone water mixture to prevailing used refrigerant R-134a was addressed to unwieldy process development in designing the ratio of mixing Acetone with water (54:1 to 76:1). The economical viability of using Acetone as primary constituent of presently developed refrigerant mixture was addressed to its lowest unit price than halogenated refrigerants. The GWP, ODP and flammability of the developed refrigerant was also moderated by designed ratio of mixing with water (54:1 to 76:1).More over the designed refrigerant was echo friendly, stable chemically & thermally, non toxic and non corrosive in nature.

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Table.1: Chemical identity specifications

IUPAC Name	Preferred IUPAC Name	Other Names
Acetone	Proan-2-One	Dimethyl ketone
		Dimethyl carbonyl
		β-Ketopropane
		Dimethyl formaldehyde
		Pyroacetic spirit (archaic)
		Ketone propane

Table.2: properties of R134a

Sl No	Properties	R-134a
1	Boiling Point	-14.9°F or -26.1°C
2	Auto-Ignition Temperature	1418^0 F or 770^0 C
3	Ozone Depletion Level	0
4	Solubility In water	O.11% by weight at 77^0 F or 25°C
5	Critical Temperature	252^0 F or 122°C
6	Cylinder Colour Code	Light Blue
7	Global warming Potential	1200

Table.3: chemical properties, structure and thermo chemistry of Acetone.

Properties	
Chemical formula	C_3H_6O
Molar mass	58.080 g·mol^{-1}
Appearance	Colourless liquid
Odor	Pungent, irritating, floral, cucumber like
Density	0.7845 g/cm^3 (25 °C)
Melting point	−94.7 °C (−138.5 °F; 178.5 K)
Boiling point	56.05 °C (132.89 °F; 329.20 K)
Solubility in water	Miscible
Solubility	Miscible in benzene, diethyl ether, methanol, chloroform, ethanol.
log *P*	-0.16
Vapour pressure	9.39 k Pa (0 °C) 30.6 k Pa (25 °C) 374 k Pa (100 °C) 2.8 m Pa (200 °C)
Acidity (p K_a)	19.16 (H_2O)
Magnetic susceptibility (χ)	−33.78·10^{-6} cm^3/mol
Refractive index (n_D)	1.3588 (V_D = 54.46)
Viscosity	0.295 m Pa (25 °C)
Structure	
Coordination geometry	Trigonal planar at C2
Molecular shape	Dihedral at C2
Dipole moment	2.91 D
Thermo chemistry	
Heat capacity (*C*)	125.45 J/(mol· K)
Std molar entropy (S°_{298})	200.4 J/(mol· K)
Std enthalpy of formation ($\Delta_fH^\ominus_{298}$)	(−250.03) – (−248.77) kJ/mol
Std enthalpy of combustion ($\Delta_cH^\ominus_{298}$)	−1.772 MJ/mol
Flash point	−20 °C (−4 °F; 253 K)
Auto ignition	465 °C (869 °F; 738 K)

temperature	
Explosive limits	2.6–12.8%
Threshold limit value (TLV)	1185 mg/m^3 (TWA), 2375 mg/m^3 (STEL)

Table.4: Thermodynamic behaviour of the refrigerant solution

T [K]	P [k Pa]	Thermal Conductivity [W/(m*K)]	State
288.70	98.000	0.1642	Liquid
288.70	4900.000	0.1667	Liquid
288.70	9800.000	0.1684	Liquid
311.20	98.000	0.1543	Liquid
311.20	4900.000	0.1581	Liquid
311.20	9800.000	0.1599	Liquid
338.10	4900.000	0.1469	Liquid
338.10	9800.000	0.1512	Liquid
340.50		0.01345	Vapour
340.50		0.0135	Vapour
340.50		0.0145	Vapour
359.00	4900.000	0.1352	Liquid
359.00	9800.000	0.1424	Liquid
362.00		0.01565	Vapour
362.00		0.01582	Vapour
362.00		0.0165	Vapour
372.30		0.01721	Vapour
372.30		0.0174	Vapour
372.30		0.01742	Vapour
391.00	4900.000	0.1239	Liquid
391.00	9800.000	0.1291	Liquid
397.00		0.0198	Vapour
397.00		0.01981	Vapour
397.00		0.01985	Vapour
423.00	4900.000	0.1112	Liquid
423.00	9800.000	0.1158	Liquid

436.70		0.0236	Vapour
436.70		0.0237	Vapour
454.30		0.02478	Vapour
454.30		0.0248	Vapour
454.30		0.0260	Vapour
463.90	4900.000	0.0966	Liquid
463.90	9800.000	0.1032	Liquid
470.00		0.02718	Vapour
470.00		0.0272	Vapour
488.50	4900.000	0.0894	Liquid
488.50	9800.000	0.0959	Liquid
494.30	4900.000	0.0898	Critical Point
494.30	9800.000	0.0965	Liquid
498.00		0.0307	Vapour
498.00		0.03071	Vapour
498.30	4900.000	0.0903	Critical Point
498.30	9800.000	0.0969	Liquid
502.40	4900.000	0.0921	Critical Point
502.40	9800.000	0.0956	Liquid
504.00		0.03085	Vapour
504.00		0.0311	Vapour
504.00	4900.000	0.0997	Critical Point
506.80	4900.000	0.1202	Critical Point
508.50	4900.000	0.1956	Critical Point
508.50	9800.000	0.0959	Liquid
509.90	4900.000	0.0939	Critical Point
513.80	4900.000	0.0697	Critical Point
516.80	4900.000	0.0566	Critical Point

522.40	4900.000	0.0544	Critical Point
522.60		0.0337	Vapour
522.60		0.03375	Vapour
534.60		0.0340	Vapour
534.60		0.0346	Vapour
535.70	4900.000	0.0471	Critical Point
548.50		0.0356	Vapour
548.50		0.0357	Vapour
553.70	4900.000	0.0498	Critical Point
557.90		0.0368	Vapour
557.90		0.0371	Vapour
571.70		0.03835	Vapour
571.70		0.0384	Vapour
571.70		0.0385	Vapour
572.70	4900.000	0.0544	Critical Point

Table.5: Global warming potential of various hydrocarbons

Organic compound/study	GWP^{CH4}	GWP^{O3}	GWP
Ethane (C2H8)	2.9	2.6	5.5
Propane (C3H8)	2.7	0.6	3.3
Butane (C4H10)	2.3	1.7	4.0
Ethylene (C2H4)	1.5	2.2	3.7
Propylene (C3H6)	-2.0	3.8	1.8
Toluene (C7H8)	0.2	2.5	2.7
Isoprene (C5H8)	1.1	1.6	2.7
Methanol (CH3OH)	1.6	1.2	2.8
Acetalhyde(CH3CHO)	- 0.4	1.7	1.3
Acetone(C_3H_6O)	0.3	0.2	0.5

Table.6: Thermodynamic behavioural comparison of Acetone with other refrigerants

Refrigerant	T_{boil}	P_{cond}	T_{crt}	P_{crt}	T_{max}	ODP	GWP	Type
Acetone	56	0.38	234.9	46	276	---	---	Wet
Ethanol	78	0.11	241.5	62.68	376	---	---	Wet
R11	23	1.26	197.9	44.07	351.8	1	4600	Isentropic
RE245fa2	28.89	1.04	171.7	34.33	226.8	0	825	Dry
R365mfc	39.82	0.69	186.8	32.66	226.8	0	825	Dry
R601a	27.4	1.09	187.2	33.78	226	0	˜20	Dry

Table.7: Comparative performances of R-134a and Acetone water mixture refrigerant

Evaporator/ temperature set	Refrigerant	T_{fz} (0C)	T_{ff}(0C)	W_k(w)	P_e(bar)	P_c(bar)	COP
Original/Minimum	R-134a	-31.3	-12.5	93.3	0.6	10.9	1.06
	$C_3H_6O+H_2O$	-30.8	-11.4	92.7	0.4	10.1	1.0
Original/ standard	R-134a	-20	4.4	127.1	0.8	12.4	1.21
	$C_3H_6O+H_2O$	-19.6	4.0	126.8	0.7	11.9	1.18
EFA/Minimum	R-134a	-30	-11.6	92.8	0.5	10.8	1.04
	$C_3H_6O+H_2O$	-29.8	-10.9	92.3	0.5	10.6	1.02
EFA/standard	R-134a	-19.1	3.6	123.0	0.8	12.2	1.17
	$C_3H_6O+H_2O$	-18.9	3.4	122.8	0.7	11.9	1.08

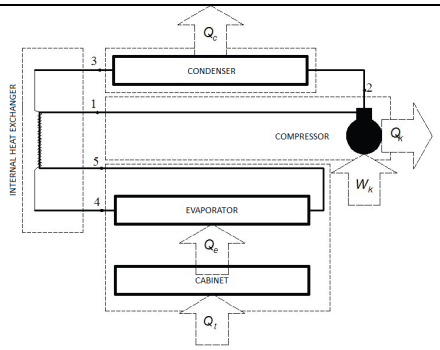

Fig.1 Flow diagram of the refrigerant test rig

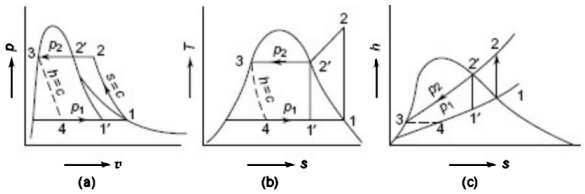

Figure.2 Flow diagram of different processes

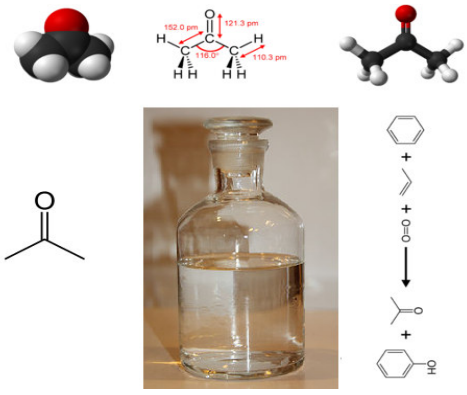

Figure.3 Structural geometry of Acetone

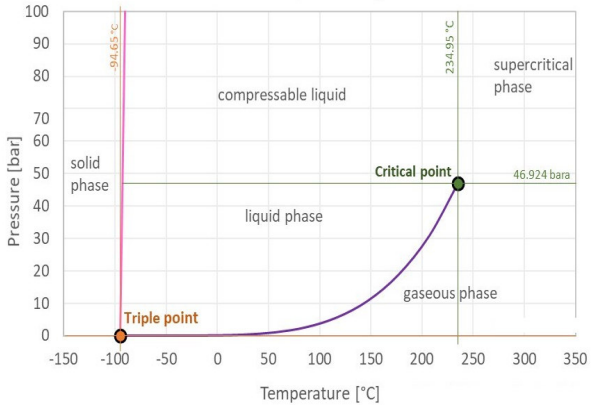

Figure.4 Phase change with temperature & pressure

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REVIEW ARTICLE

Nutrient Management in Foxtail millet: A Review

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ABSTRACT

Foxtail millet (*Setaria italica* L.), like other small millets belongs to the family Poaceae, is drought tolerant crop grown in drylands under rainfed conditions with higher CO_2 abatement opportunities. In the present context of temperature rise and ill effect of climate change, the low input demanding and ecologically sound foxtail millet can automatically be chosen for agricultural sustainability in drylands. Foxtail millet is nutritionally superior to other cereals. Recently developed varieties of foxtail millet respond well to added nutrients and proper nutrient management is essential for production sustainability. In the present paper, the available literature on different options of nutrients application to foxtail millet for sustainable productivity is reviewed. Application of nitrogen in the soils with low available nitrogen is beneficial for enhancing productivity. Nitrogen in combination with phosphorus or recommended dose of balanced fertilizer can boost the yield of foxtail millet. For sustainable production of foxtail millet, integrated nutrient management can be adopted. As there is insufficiency in research and the crop is having nutritional and ecological importance, there is ample scope for future research towards precision nutrient management.

Keywords: Nitrogen, Application, research, foxtail millet,

INTRODUCTION

Millets are a group of coarse cereals that produce small seeds and used mainly as food, feed and forage grown in arid and semi-arid regions in the world. Amongst different millets, sorghum (*Sorghum bicolor* L.) and pearl millet (*Pennisetum glaucum* L.) are known as major millets, however, rest are categorized as small millets. Under fragile ecological conditions, small millets are cultivated by resource-poor farmers in subsistence cropping system with an acreage of around 7.0 lakh ha with a productivity of 633 kg/ha (Maitraand Shankar, 2019). In India, small millets are grown in 6.8 lakh ha and the country ranks the first with 80% of the production of Asia (Maitra, 2020). Out of different small millets cultivated in India, finger millet (*Eleusine coracana* L. Gaertn) shares about 80% of production

and it is followed by *kodo* millet (*Paspalum scrobiculatum* L.) and foxtail millet (*Setaria italica* L.). Foxtail millet, like other small millets, belongs to the family *Poaceae*,is highly drought tolerant crop grown in drylands under rainfed conditions with higher CO_2 abatement opportunities (Brahmachari *et al*., 2018). In India, the cultivation of foxtail millet is confined mainly to Andhra Pradesh, Karnataka and Tamil Nadu. The nutritional value of foxtail millet is highly appreciating as 100g of foxtail millet grain contains fibre 8 g, protein 12.3g; carbohydrates 60.9g, fat 4.3g, calcium 31mg, iron 2.8mg, phosphorus 290mg, vitamins 3.3g, minerals 3.3g and food energy 323-350 K Cal (Vanithasri*et al*., 2012). Besides, small millets are considered as functional foods containing bioactive ingredients useful to combat against chronic diseases (Banerjee and Maitra, 2020). In the present context of adverse climatic conditions due to global warming, dryland agriculture became more risky and growing of hardy crops is one of the solutions to combat climate change. Foxtail millet is a low input demanding and ecologically sound crop which can automatically be chosen for agricultural sustainability in drylands. The average productivity of foxtail millet in India is 780 kg ha^{-1} (Monisha *et al*., 2019). But under proper agronomic management, the crop can produce about double of its yield in unit area as evidenced in experimental results (Ramyasri *et al*., 2018; Mubeena *et al*., 2019). Sufficient research work has not been carried out on nutrient management in foxtail millet for maximization of productivity. Based on published literature, an initiative has been taken up to gather information together on nutrient management in foxtail millet targeting production sustainability.

Nutrient Management Options

Foxtail millet is a low nutrient demanding crop, but during recent times improved varieties have been developed which respond well to applied nutrients. In comparison to major cereals, much information on nutrient management in foxtail millet is not available for different agro-climatic zones under different cropping system. Researchers suggest adopting integrated nutrient management (INM) for different crops. The INM is proportionate use organic manures, biofertilizers and chemical fertilizers. The combined and harmonious use of nutrients from different sources in INM enables the sustainable agricultural production system by enhancing soil fertility, water holding capacity and soil microbial activity with a holistic impact on soil physico-chemical and biological properties (Maitra *et al*., 2019).

Chemical Fertilizer

Nitrogen and phosphorus

Nitrogen (N) is one of the essential primary nutrients that influence growth and productivity of crops including foxtail millet. N is the component of the proteins and useful for the function of chlorophyll, various enzymes, nucleic acids and indispensable organic compounds (Ohyama, 2010; Aczel, 2019). To provide N, generally chemical fertilizers are applied to crops. NavyaJyothi*et al.* (2016)observed that application of 50 kg N ha^{-1} increased growth and productivity of foxtail millet in a trial conducted at Tirupati, Andhra Pradesh in sandy loam soil with low available N.Nandini*et al*. (2018) noted that application of 125% recommended dose of nitrogen (RDN) expressed better performance of yield attributing characters like number of effective tillers, panicle length, panicle weight and test weight of foxtail millet at Shivamogga, Karnataka in typical red sandy loam textured soil of with slightly acidic in reaction and low available N.

The results revealed that 125% RDN registered significantly more grain and straw yields and protein content of seed than 100% RDN, but 100% N resulted in more crude fibre content in seed. Further, a field experiment carried out duringrabi season in rice fallows at Naira, Andhra Pradesh in neutral sandy loam soil with low available nitrogen showed that application of 80 kg N ha^{-1} produced more grain (1684 kg ha^{-1}) and straw (3101 kg ha^{-1}) yields of foxtail millet and higher N uptake than lower doses(Ramyasri*et al*., 2018). Phosphorus (P) is a vital nutrient which triggers plant growth and development. In process the photosysthesis, adenosine triphosphate (ATP) is produced which is the energy unit of plants and P is there in the structure of ATP. Like N, applied P increased yield of foxtail millet as noted in different experiments. In the alfisols of Karnataka, the application of 30 kg N+15 kg P_2O_5 ha^{-1} gave higher grain yield (1792 kg ha^{-1}) which was followed by 22.5 kg N+11.25 kg P_2O_5 ha^{-1} which yielded grain of 1615 kg/ha

(Naik*et al*. 2010).Reddy *et al*. (2019)observed a synergistic effect of N and P and application of 60 kg N ha^{-1} and 40 kg P_2O_5 ha^{-1} resulted in highest growth, grain and straw yield as compared to other treatments under south Odisha conditions.

Combined Application of nitrogen, phosphorus and potassium

The proportionate use of three primary nutrients, namely, N, P and K is known as balanced fertilization to crops. As per the soil fertility status balanced application of these three major nutrients are recommended to obtain optimum productivity of crops. Researches were carried out on application of N, P and K in foxtail millet which indicated that application of balanced fertilizer enhanced productivity (Hasan*et al*. 2013). In medium black soil of Raichur, Karnataka foxtail millet recorded significantly higher grain and straw yields and nutrient uptake with the application of 100% recommended dose of fertilizer (RDF) than 75% and 125% of RDF (Mubeena *et al*., 2019).

Organic Manures and Biofertilizers

Organic manures supply almost all essential nutrients to crops, but the analytical value is less. During the present time, there is substantial growth in organic farming with an increasing demand of organically produced foods. In organic farming, different organic manures and biofertilizers play an important role to supply nutrients to crops. Research evidences indicated that organic manures and biofertilizers enhanced productivity of foxtail millet significantly. Upendranaik *et al*. (2018) observed that a combination of different organic manures along with mulching increased growth and productivity of foxtail millet. Application of *jeevamrutha* + mulching + IFS compost + vermicompost + *panchagavya* resulted in significantly more grain yield of foxtail millet over control at Raichur, Karnataka. Rafi *et al*. (2012) and Rafi and Charyulu (2016) reported that inoculation of *Azospirillum* sp. and phosphate solubilizing bacterium (PSB) individually and combined inoculation improved the yield of foxtail millet.

Integrated Nutrient Management

Integration of organic manures, inorganic fertilizers and biofertilizers play an important role in enhancing crop productivity, sustaining a soil health and reducing adverse effects on environment. Research trials carried out on INM indicated positive impacts on productivity of foxtail millet. A field experiment conducted at Sundarbazar, Nepal, clearly indicated that INM resulted in enhancement of productivity of foxtail millet and application of FYM 6 t ha^{-1} along with NPK 60:30:20 kg ha^{-1} gave 152% more yield than control (Ojha*et al*., 2018). In another experiment, application of 50% RDF + 25% N as neem cake + *Azophos* recorded maximum values in expression of plant height, number of tillers, panicle length, Test weight, grain and straw yield in sandy loam read soils at Madurai, Tamilnadu and the treatment was superior to 100% RDF (44:22:0 kg N:P_2O_5:K_2O ha^{-1}) and absolute control (Monisha*et al*., 2019).However, Kumaran and Parasuraman (2019) recorded that integrated nutrient management increased grain yield of foxtail millet at Tiruvannamalai district of Tamilnadu and combined application of farmyard manure, recommended dose of fertilizer and foliar application of 3% Panchagavya at 20 days after sowing gave the maximum grain yield (1652.5 kg ha^{-1}). A combined application of 75% RD N through Urea + 25% N through PM + *Azospirillum* Seed Inoculation gave maximum grain yield (2.31 t ha-1), higher net return and maximum B:C ratio (2.59) at Prayagraj, Uttar Pradesh in sandy loam soil (Selectstar Marwein *et al*., 2019).

Future Scope of Research

Chemical fertilizer production process releases enough of GHGs causing global warming and there is urgent need for prevention of wastage and increase on nutrient us efficiency. The study reveals that enough research has not been conducted on efficient nutrient management of foxtail millet. But nutrient management is one of the key aspects determining productivity. Hence the future research may be carried out in the following directions.

1. Study may be intensified on INM in different agro climatic regions under various cropping systems.
2. Research work may be laid out on management of secondary nutrients and micro-nutrients in foxtail millet. Moreover, time and method of nutrient application should be considered.

3. There is enough potential for adoption of precision nutrient management technologies like soil test crop response (STCR), site specific nutrient management (SSNM),diagnosis and recommendation integrated system (DRIS) on to enhance nutrient use efficiency with target yield output. Further, latest precision technologies like use of geographic information System (GIS), sensors and hyper-spectral imagery may also be considered in future research for detection of nutrient stress in plants, geochemistry of soil and precision crop management (Hakim *et al*., 2016; Bogue, 2017; Robinson and Kinghan, 2018).

CONCLUSION

As foxtail millet is cultivated in low fertility soils of drylands with improper management practices, fertilization plays a pivotal role for increasing the crop yield. INM is considered as one of the best approaches for production sustainability of foxtail millet. The available literature indicated some limitations like insufficient research on INM for different agro climatic zones and precision nutrient management and the present study suggests future research scope for sustainable foxtail millet production.

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RESEARCH ARTICLE

Impact of Fly Ash and Vermicompost Treated Soil on Growth of *Vigna radiata* L. and *Cicer arietinum* L.

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ABSTRACT

In this study, the growth of green gram (*Vigna radiata* L.**)** and chickpea (*Cicer arietinum* L.) were evaluated in different soil conditions. Soil, vermicompost and fly ash in different proportions were taken to observe the impact of flyash and vermicompost on shoot length of these two species. All the growth attributes was found to be maximum in plants grown in the plot with soil and vermicompost for both these pulse crop. The length of chick pea plant grown in soil and vermicompost in 4: 1 ratio was maximum with 26.9cm in 3rd week after germination of the seeds. The growth of green gram was measured and maximum growth of 18.8cm was found in soil and vermicompost with 3: 2 ratio respectively and SVF (Soil + Vermi compost + Fly ash) with 17.7cm and 1:3:50 ratio showed no growth and ultimately all plants died. The present study was undertaken to observe the impact of fly ash and on the growth and yield of green gram and chickpea.

Keywords: *Cicer arietinum* L., Fly ash, growth, soil fertility, vermicompost, *Vigna radiata* L.

INTRODUCTION

Green gram

Green gram is the most important pulse crop in the sub-tropical zones of the world. It contains 51% carbohydrates, 24 to 26% proteins, 3% vitamins (Afzal et. al., 2008). Besides providing protein in the diet, greengram has the remarkable quality of helping the symbiotic root *Rhizobium* to fix atmospheric nitrogen (Anjum *et.al.,* 2006). Still several works are going on to study the crop growth and also alternate uses of fly ash and the performances of the pulse crop (Hassan *et.al.,* 2004). The yield depends on soil codition, time of sowing, climatic condition and also the crop varieties (Anjum *et.al.,* 2006). The rate of growth varies depending upon these factors. It was also revealed that plant with optimum leaf area may produce higher yield (Pandey et.al 1978; (Dutta and Mondal 1998). A plant with

optimum leaf area and net assimilation rate may produce higher biological yield. Green gram has been consumed as a common food in china for more than 2,000 years. It is well known for its detoxification activities and it uses to refresh mentality, reduce swelling in the summer .it is beneficial in the regulation of gastrointestinal in the upset and to moisturize the skin (Min, 2001).

Chick pea

Cicer arietinum L. was first domesticated in the Middle East. It is widely in India, Australia, Pakistan, turkey. It is important cool season pulse crop and is also called as Bengal gram. I terms of pulse production India contributes total 255 to the world pulse production (Pooniya *et.al*., 2015). Chick pea is the premier crop in India and grown on 8.25 million hectares during 2014-2015 resulting 7.33 million tones yield. This accounts for about 70% of the total global area with 67% of global production (Anonymous, 2016). Chickpea is an important source of protein in the diet of the poor & is particularly important in the diets and is an important substitute for animal protein. It is an excellent source of protein of about 18 to 22%, carbohydrates from 52 to 70%, fat (4 to 10%) and minerals, like calcium, phosphorus, iron etc. and also contain vitamins (Prasad, 2012).

MATERIALS AND METHODS

The present research work conducted at the field of Centurion University campus, Bhubaneswar, during the period of September to December 2019. The field experiment were conducted to compare the growth rate of green gram and chickpea seeds in different soil condition and its impact on vegetative growth and yield of green gram and desi chickpea.

Pot preparation

Before sowing of the seeds, the pods were prepared. Eight pots prepared for sowing the seeds. Vermi compost, fly ash was added in the needed quality. Soil, vermicompost and fly ash were mixed in different proportion and filled in earthen pots(20 cm diameter and 28 cm height) Before filling the pots small broken pieces of stones were placed on the bottom of the pot for free drainage.

Soil testing

Soil testing is an important practice to know the soil in which the crop will be grown. Soil testing is done to optimize crop production and to known the nutritional content of the soil and improve the nutritional balance of the growing media. Soil samples of different pots were collected before the addition of manure to the soil. Vermi compost, soil and fly ash in different ratios i.e. soil and vermin compost in 3:2 ratio, soil and fly ash(20 gm),soil ,vermin compost and fly ash in 3:2:10 gm ratio, soil, vermi compost and fly ash in 1:3:50 gm ratio. These ratios of pods are prepared for green gram. Then soil, vermi compost and fly ash in 3:2:10 gm ratios, soil and vermin compost in 4:1 ratio, soil, vermi compost and fly ash in 2:2:50 gm and last only soil and few vermin compost for desi chickpea.

Crop/planting material

The variety of green gram and desi chickpea were used for the present study. The required seeds were collected from the market. Healthy, well matured seeds were selected. Before sowing the seeds were tested for germination was found to be over 90%. The important characteristic of two varieties was enumerated. Green gram and chickpea are medium statured, semi erect cultivars with basal primary branches. Stem pigmentation is absent at the seedling stage, but green gram becomes light green at the late vegetative stage and chickpea become light radish at the late vegetative stage respectively. Leaves are dark green with slightly pubescence. Leave size is medium with dark green colour, short petiole and rachis that form no tendrils. The flowers of green gram are light green and flowers of chickpeas are light pink. For sowing of seeds, wild type seeds are collected. Seeds sown were done in pots using traditional hand sowing method. Dry land was required for germination. Seeds were both sown in random traditional way and in lines.

Cultivation Practices

Vermi compost and fly ash were added in different concentrations. Thinning and weeding were done at 20 days after sowing, when the plant attained after 15 days of sowing. Distance between the plants was maintained at a gap of each 7 days. Second weeding was done at 35 days, when the plants attained after another 7 days gap. For crop sampling and data collection, the plants were selected randomly from each pot and were uprooted for data recording. Plant height of 10 plants was randomly measured in weekly interval. Plant height was measured randomly from each pot from the ground level to the apex of the main shoot of the plant by meter scale.

RESULTS

The growth of green gram and desi chickpea in different proportion of soil, vermicompost and fly ash were studied. Data depicted in Table 1revealed that the growth of chick pea plant grown in soil and vermicompost in 4: 1 ratio was maximum with 26.9cm in 3rd week after germination of the seeds. These plants also bear flowers. SVF (Soil + Vermi compost + Fly ash) in 3:2:10 ratio showed 25. 7 cm. followed by SV (Soil + Vermi compost) in 3: 2 ratio, in SVF with 2:2:50 ratio, showed no growth after 3rd week. All the plants died in SF with 1:20 ratio after 3rd week. The growth of green gram was measured and maximum growth of 18.8cm was found in soil and vermicompost with 3: 2 ratio respectively and SVF (Soil + Vermi compost + Fly ash) with 17.7cm and 1:3:50 ratios showed no growth and ultimately all plants died (Table 1, Fig. 1). Under such condition, the productivity of soil can be sustained at satisfactory level by use these biofertilizers.

In 1st pot we take the composition of soil and vermi compost in 3:2 ratios. The length of green gram seedlings was 9. 7 cm in 1st week. Because the composition is suitable for the growth of plants.nut in 2nd week growth of some plants did not occur because some nutrient present in the soil inhibits the growth and finally in 3rd week which plants are exist they grows 18.8 cm. In 2nd pot we take the composition of soil and fly ash in only soil: 20 gm fly ash ratios. The plant of mung bean grows 9. 7cm in 1st week. But in second week no growths occur. Because the composition is not suitable for the plants so they inhibit the growth. In 3rd week all were found to be died. In 3rd pot we take the composition of soil, compost and fly ash in 2:2:10 gm ratios. The seedlings showed 9. 7cm in length in 1st week, 13.4cm in 2nd week and 17.7 cm in 3rd week. In 5th pot the composition of soil, compost and fly ash is 3:2:10 gm. This composition was found to be suitable for the growth of chickpea plants. In 1st week, the length of plants was 10.2 cm, in 2nd week 16.7 cm and 3rd week 25.7cm respectively.

In some pots flowers emerged. In 6th pot the composition of soil and compost in 4:1 ratio showed maximum growth in length in which the seedling length in 1st week was10.3cm, 2nd week 17.9cm and 34rd week 26.9cm respectively. In 7th pot the composition of soil and fly ash was 2:2:50 gm ratios. In 1st week plant growth is 4 cm, 2nd week 10 cm and 3rd week no growths occur. In 8th pot the composition of soil and fly ash is 1:20 gm in 1st week plant growth is 8.2cm, 2nd week 10.3cm and in 3rd week no growth in length was noticed rather all seedlings died because the growth was inhibited by the minerals present in this composition leading to death of the seedlings.

DISCUSSION

Number of pods per plant was found to be highest in the plants grown in soil treated with fly ash and vermi compost.Root nodules are also found to be increased in the plants treated with the vermi compost.it was reported that the vermi compost is more beneficial than that of fly ash.In the composition of 2:2:10 gm the plant of mung bean grow well.but in the ratio of 1:3:50 gm the plants dies due to excess amount of fly ash.

CONCLUSION

This experiment revealed that fly ash can be mixed with the soil in minimum doses with vermicompost for cultivation of crops. But the pulses should be evaluated for their nutritional composition to estimate the trace

element and heavy metals. From these results it can be summarized that the plant growth depends on the status of soil, variety and also other abiotic factors including climatic condition.

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Table 1. Soil composition and seedlings growth/week in *C. arietinum* L. and *V. radiata* L.

Treatments	Soil Composition	Composition Ratio (gm)	Length of the plant (Cm)			Remarks
			1st Week	2nd Week	3rd week	After 3rd week
T_1	SV	3:2	9. 7	13.4	18.8	flowers appeared
T_2	SF	1:20	9.1	9.1	Died	All plants died
T_3	SVF	2:2:10	8.5	13.6	17.7	Stunted growth
T_4	SVF	1:3:50	9. 2	13 .1	No growth	All plants died
T_5	SVF	3:2:10	10. 2	16 .7	25.7	flowers appeared
T_6	SV	4:1	10.3	17. 9	26.9	flowers appeared
T_7	SVF	2:2:50	8.2	10.3	No growth	Stunted growth
T_8	SF	1:20	5.5	5.5	All died	All plants died

*SV: Soil + vermi compost; SF: Soil + fly ash; SVF: Soil + Vermi compost + Fly ash; T_1- T_4 : Green gram; T_5- T_8: Desi chickpea

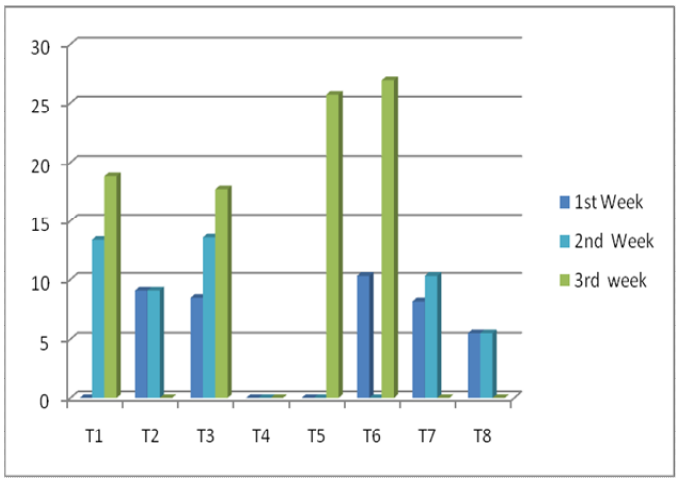

Fig. 1 Growth (length in cm/week) of *Cicer arietinum* L. and *Vigna radiata* L. seedlings

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RESEARCH ARTICLE

Basic Design to Build the Airship for Indoor Application

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ABSTRACT

This work describes the conceptual design study before the detail designing, fabrication and testing of the airships. The airship is planned to design for indoor flight for 30 minutes with taking a payload of 0.5kg and flying at a constant altitude. This report provides the standard methodology for RC airships, basic buoyancy, aerodynamic calculations and structural envelope considering four basicflight parameters such as takeoff, hover, cruise and landing. The theoretical force analysis was done by definding maximum speed, cruise altitude and takeoff time. The thrust required in each flight regime was then determined based on calculation of the lift, weight and drag forces. The conceptual design was done by taking five concepts for the envelope shape to find out the optimal shape of airship. An iterative procedure was developed to optimise the envelope design based on the weight of components and the lifting force needed to achieve neutral buoyancy.

Keywords: Airship, Blimp, Conceptual design, Airship envelop

INTRODUCTION

Aircraft can be divided into two groups: lighter-than-air aircraft (LTA) and heavier-than-air aircraft (HTA) [1]. Conventional fix-wing and rotation-wing aircraft which utilize lifting surfaces like wings and blades as the source of lift belong to HTA. LTA is mainly referring to aircraft such as balloons and airships (blimps). Unlike HTA, LTA is designed to contain within their structure a sufficient volume of gas lighter than air (heated air, hydrogen, or helium)

to acquire enough lift force from the buoyancy of the gas. Without consuming extra fuel to generate necessary lift for floating, airships over advantages over air cargo transportation in the past.

Many different types of aircraft are designed and fabricated for diverse applications and scenarios. A survey of recent developments in aerial robotics gives a general overview of the definition, types, categories, and topics of aerial robotics[2]. This work describes classifies and briefly introduced more than one hundred high-quality aircraft papers from more than thirty thousand that have been published in the top journals and conferences in a systematic way. In the last 50 years airships have been used for certain niche applications such as advertising, surveillance and aerial photography. The most well known advertising craft is the Goodyear blimp which has been prominent at major sporting events. Smaller craft have been used for advertising and photography in large indoor arenas such as basketball and ice hockey stadiums. The United States Coast Guard has also experimented with using airships for high altitude surveillance of its borders and coastline.

Some earlier scientific and technical notes and documents about airship design can be found as technical reports from NASA. There are two famous reports by Tuckerman [3] [4], emphasizing two most critical issues of airship design - the determination of forces on an airship hull and inertia factors. Regarding airship, [5] introduced the recent researches and conceptual designs of airships and classifies the airships according to its body. In paper [5], a state-of-the-art literature review on airship dynamics modeling is presented, aerodynamics and flight dynamics modeling method are described. This also provides the structural flexibility, incorporation of atmospheric turbulence as well. Based on six degrees of freedom, an attractive dynamic model is presented in ref. [6]. In ref.[7], a blimp-based robot and its navigation system are introduced. The blimp is a commercial kit which can be used as platform directly. Ref. [8] introduces a design methodology and fabrication of an easily deployable finless airship for indoor surveillance and advertisement. The detailed and step-wise procedure for designing and fabricating indoor remotely controlled airships are discussed in [9].

A comparison between the airships using design methodology introduced in this work with some other commercially available airships are also exhibited. Paper [10] introduces an airship that mimics fish-like movement in the air, propelling an airship by undulating its hull and a caudal fin. A work on DEA predicted that DEA strip actuators could reach 90% maximal efficiency in optimal conditions. However, an actual peak efficiency of 18% was measured in the experiment due to the high energy loss of such a voltage transform [11]. The propulsion efficiency analysis of fish-like robot is exhibited in [12], the relationship of speed and energy efficiency are analyzed. Ref. [13] does a research on the efficiency of fish propulsion. As a commonly used propulsion unit for indoor airships, small-diameter propellers performance data including energy performance are tested and a reliable database of performance data of many propellers has been created in [14]. Recent years, several fish-like indoor airship projects appeared due to high efficiency of fish propulsion. [15] [16] the propulsion efficiency of both propeller and fish movement is studied. The efficiency of fish movement and propeller is studied in [17] and [18] respectively.

Aims

The project aims to design and construct a small airship capable of indoor flight.
Specifically, this project aimed to achieve three main objectives:

- To design and build an airship to meet specified flight parameters
- To implement a complete manual and partial automatic control system
- To have the ability to capture images and transmit them to the ground

The final product could be used for indoor aerial photography, surveillance and advertising purposes. This paper discuses only the conceptual design part for a airship of following requirements.

CONCEPTUAL DESIGN

Desired Modes of Flight: The modes of flight describe the rotational and translational movement of the airship. The requirements of each flight mode were determined based on the feasibility study [20] and the broad goals of the project.

Maneuverability: The manoeuvrability of an airship is described using a right handed, orthogonal coordinate system passing through the airship's centre of volume (Figure 1). If a force acts on the airship it causes a turning moment which is defined as "the product of the magnitude of the force and of the perpendicular distance from the Cv to the line of action of the force" (Beer and Johnston, 1987). The three possible turning moments of an airship are classified as roll, pitch and yaw moments about the x, y and z axes respectively. Control of yaw and pitching moments was part of the project definition, but roll control was not deemed necessary. As almost two thirds of the mass is contained in the gondola any minor roll moments will be counter-balanced by the natural tendency of the airship to move back to the equilibrium position. The rate of turn of the airship describes how fast the airship can yaw. The feasibility study suggested that it would be possible to achieve a 90º turn in 3 seconds. The target rate-of-turn, was therefore 30º/s.

Takeoff: The takeoff manoeuvre describes how the airship moves from the ground to its cruise altitude. The takeoff motion is designed to be entirely vertical, although it is also possible to takeoff diagonally with a small thrust from the side fans. Diagonal takeoff is not an essential part of the project. Two flight parameters needed to be determined so the takeoff mode could be defined accurately. A cruise altitude of 6m was chosen mainly due to a limitation in the ultrasonic height sensors which fail to accurately measure height above this altitude. The time required to reach the cruise altitude also needed to be defined. Preliminary thrust and drag calculations suggested that 20 seconds was an achievable ascent time hence this figure was chosen.

Hover: When the airship does not move in the horizontal plane and maintains its altitude it is in hover mode. Hovering mostly occurs at the cruise altitude. As a safety mechanism, the airship was designed to be slightly less than neutrally buoyant, that is the lifting force is almost that of the overall weight force. Therefore, to hover, a constant upward thrust is required to maintain altitude. The magnitude of the upward thrust will be more closely defined in the detailed design.

Cruise: The cruise mode is essentially the same as the hover mode except that it includes movement in the horizontal plane. Cruise calculations required that two flight parameters be determined. A maximum cruise speed of 1.0 ms-1 was deemed to be achievable based on the initial thrust and drag calculations. The performance of the NUS airship and the Rowan University airship also suggested that this cruise speed was appropriate. To calculate the maximum cruise thrust, the time to reach maximum speed also needed to be defined. A value of 10 seconds was chosen based on preliminary testing of ducted fan units.

Landing: The landing of the airship was designed to be entirely vertical although there is the capability for a descent where horizontal thrust is provided. Since the total weight of the airship is designed to exceed the lift provided by the helium, the airship should descend under its own weight. Descent time from the cruise altitude was designed to be less than 20 seconds. The excess weight calculations will be used to determine the exact theoretical descent time. Summary of Flight Parameters is given in Table 3.

FORCE ANALYSIS

Weight Determination: The exact weight of the airship was difficult to ascertain during the conceptual design phase. Research was done into the weight of every component and an overall weight estimate was made.The

envelope and stabiliser weights were estimated based on discussions with the manufacturer of the envelope, Airship Solutions. They provided information on the polyurethane density and thickness. This was then combined with preliminary surface area estimations to calculate the total weight of the envelope. It was especially difficult to estimate the weight of the gondola housing and internals as the gondola design changed frequently. The balsa wood density and thickness were combined with an approximation of the total surface area of the gondola to estimate its weight. The weight of the motors, ducted fans, batteries, speed controllers and automatic control components was determined from manufacturer data sheets. Parts that were definitely going to be needed in the final design were purchased and then weighed to confirm the manufacturer's data.

Lift Determination: The lifting force is comprised of the static lift from the helium and the dynamic lift created by the pressure distribution around the airship during flight. The envelope is very inefficient in creating dynamic lift due to its shape and the low speed airflow. The dynamic lift was assumed to be negligible compared to the static lift.

Lifting gas: From Archimedes' principle, the upward buoyancy force due to the lifting gas is equal in magnitude to the weight of the fluid (air) displaced. To be effective in generating lift, the density of the gas displacing the air must be as low as possible. The buoyancy force can be expressed as a function of the lifting gas density, air density and the volume.

$$F_{Lift} = (\rho_{air} - \rho_{lifting\ gas})\, g\, V$$

Where

F_{Lift} = Lifting Force (N)
ρ_{air} = Density of Air (kg/m^3)
$\rho_{lifting\ gas}$ = Density of Lifting Gas (kg/m^3)
V = Volume of the Envelope (m^3)

Four alternative lifting gases could have been used for the airship: hydrogen, helium, methane and ammonia. A comparison of the lifting force is shown in Figure 2 and the calculations for each gas are shown in Appendix B. The unit of lifting force was converted to grams for ease of comparison with the mass of components. Figure 2 shows that to lift 3kg of weight using ammonia or methane would require a volume of at least 5m3. Hydrogen and helium provide almost double the lifting force per volume and hence would need a total volume of approximately 3m3. Hydrogen could not be used due to its extreme flammability. Hence it was concluded that helium was the only suitable gas for the airship.

Atmospheric Effects: Temperature, altitude and air density all affect the lifting capacity of the airship. Due to the low ceiling height, any altitude affects were deemed negligible. Air was assumed to be an ideal gas and hence the affect of temperature on the air density can be calculated.

$$\rho_{air} = \frac{P \cdot M}{R \cdot T}$$

Where:

P = atmospheric pressure (Pa)
M= Molar mass of air (kg/kmol)
R= Specific Gas Constant (N m kg^{-1}kmol^{-1})
T= Temperature (K)

The lifting force was then determined at varying temperatures by substitution into the lift equation. The complete solution can be seen in Appendix B. As the airship was designed for indoor use, the temperature would generally be between 15 and 25º C. The maximum operating temperature for the airship was determined to be 35º C (950g of lift

per m3). At higher temperatures, the helium lifting force was insufficient for the airship to fly.

Thrust Determination: Using the flight parameters established in section 3.1 it was possible to calculate the thrust needed in each flight mode. The thrust required was calculated in grams as this is the standard unit used for rating RC ducted fans.

Takeoff: In takeoff mode the airship must overcome the drag force acting downward as well as the weight force. The buoyancy force alone is not sufficient for takeoff, hence an upward thrust must be provided. The required thrust in takeoff was determined from applying Newton's Second Law to the airship. The equation assumes that the buoyancy force is equal to the weight of the airship.

$\Sigma F = m\,(dv/dt) = \text{Thrust} + \text{Buoyancy} - \text{Weight} - \text{Drag}$
$\therefore \text{Thrust} = m\,(dv/dt) + \text{Drag}$

The drag coefficient for the envelope in takeoff was conservatively approximated to be equal to the drag coefficient for a horizontal cylinder moving upward which has C = 1.15 (Munson, 2006). All other variables in the takeoff equation were defined in the flight parameters. The maximum thrust required in vertical takeoff was calculated to be 96g.

Hover: The thrust required in hover was determined using the same procedure as for takeoff mode. As stated in section 3.1, the lift force was designed to be just less than the weight force, hence a constant vertical thrust was required in hover mode. The airship was designed to descend from a height of 6m in 20 seconds. An excess weight of 20 grams was chosen as this allowed the airship to descend in approximately 20 seconds. Hence the constant upward thrust was required to be 20 grams for the airship to hover.

Cruise: In cruise mode, the airship required thrust in both vertical and horizontal directions. The vertical thrust was equal to that needed for hover. The drag coefficient was approximated as an ellipsoid with C =0.38 (Munson, 2006). The drag caused by the gondola was assumed to be negligible compared to the drag of the envelope especially considering the low maximum speed. From the hover force analysis, the constant vertical thrust was determined to be 20g. The forward thrust was calculated by applying Newton's Second Law in the horizontal direction. The required horizontal thrust was calculated to be 130g.

$\Sigma F = m\,(dv/dt) = \text{Thrust} - \text{Drag}$
$\therefore \text{Thrust} = m(dv/dt) + \text{Drag}$

ENVELOPE DESIGN

Structural Parameters: The structure of the envelope could be based on several main designs: rigid, non rigid and semi rigid. Each type of structural design was assessed based on its cost, lifting force efficiency and aesthetics. Rigid airships have an internal framework which maintains the shape of the envelope. Rigid internal frameworks are typically seen in large scale airships such as the giant Zeppelin craft of the 1920's and 30's. Several ballonets containing the lifting gas are located within the main envelope as seen in Figure 7. Separate ballonets containing air are also housed in the envelope. The weight of the envelope, and hence the lifting force, can be controlled by pumping air in or out of the ballonets. For a small airship design, a rigid structure significantly decreases the effective lift and increases the complexity and cost of manufacturing. Non-rigid airships contain no internal framework to maintain the shape of the envelope. Instead, their shape is maintained by the pressure of the lifting gas within the envelope. Larger non-rigid airships typically include a protective outer surface, made from a robust material such as rubber. Small scale designs generally use a single skin of a durable material which has a low

permeability to helium. One disadvantage of non rigid airship is that other components cannot be stored within the envelope. Non rigid envelopes are a simpler, less expensive alternative to rigid envelopes and are commonly seen in smaller airships under 10 metres in length. Semi rigid airships try to include the most desirable features from both rigid and non rigid airships. Semi rigid airships have a non rigid envelope with an internal pressure higher than that of the atmosphere, to maintain their shape. They also have a framework, but this framework in not as extensive as that found in rigid airships and hence the overall weight of the envelope is reduced. The key requirements in the design of the envelope include indoor use and a low cost. A singled skinned, non rigid design is the most suited for this project's application. It is an inexpensive option and has a high lift to weight efficiency. A non-rigid design is also the most appropriate for indoor use as forces due to air currents will be low. This style of envelope is also commonly used by projects of a similar scale and is regularly used in small commercial craft.

Shape and Aerodynamics: Using the knowledge obtained through the feasibly study, five concepts for the envelope shape were developed. These shapes are outlined in Table 3. The concepts were created using geometric formulae for hemispheres, ellipses, cones and cylinders. The aerodynamics, volume efficiency and aesthetics of each shape were then analysed. An aerodynamic analysis of the different shapes included an examination of the frontal area and the streamline properties. Both of these properties affect the form drag of the envelope. Each of the shapes was given a rank (1-5) based on how they compared with an ideal aerodynamic shape. The results of this analysis are shown in Table 4. The results show that the designs which feature taper and/or ellipsoid shapes will produce less drag.

To minimise the lift required it was important to minimise the weight of the envelope. The weight of the envelope was determined from the surface area of the material and its material properties (thickness and density). The optimal shape for the envelope would therefore have the smallest surface area while providing the same volume of helium. Using a constant volume and the geometric formulae for each shape, the surface area to volume ratio was calculated. The results are shown in Table 5. From this table it can be seen that the two shapes with the smallest surface area to volume ratio (and hence best lifting efficiency) are the "hemisphere front with elliptical end" and "different elliptical front and end". Table 5 provides the surface area to volume ratio for all of the envelope shape. The surface area to volume ratio was found to be minimum in case of "different elliptical front and end" shape. This shape was used to develop the final envelope design based on the lift requirements of the airshp.

CONCLUSIONS

The aim of this work was to make a conceptual design for structural and aerodynamics envelope. This methodology for conceptual design for a small airship was found to be very useful shape of design of the airship. It was not only covers the basic aspects of airship design but also governs the various options that can be utilized depending on the user constraints. However, there still lies a tremendous scope for improving the current design from the aerodynamic point of view. Also further work is required for the dtaile design and the fabrication of this airship for this scope of project. Using the knowledge obtained through the feasibly study, five concepts for the envelope shape were developed. The concepts were created using geometric formulae for hemispheres, ellipses, cones and cylinders. The aerodynamics characterstics and volume efficiency of each shape were analysed. It was found from study that "Different Elliptical Front and End" envelop shape was optimal envelope shape. Surface Area to volume Ratio of this shape was found to be 3.4 which is minimum compare with other different type of envelope.

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Table 1. Airship Characteristics

Category	Value
Payload weight	0.5 kg
Cruise Speed	1 m/s
Time of Flight	60 mins
Cruise height	8 m

Table 2. Maneuverability Requirements

Manoeuvre	Control
Yaw	Controlled manually
Pitch	Controlled automatically

Table 3. Flight Parameters

Parameter	Value
Cruise Altitude	6 metres
Takeoff time to reach cruise altitude	20 seconds
Maximum Yaw rate	30º/second
Maximum Cruise speed	1 1 metre/second
Time to reach max cruise speed from rest	10 seconds
Descent time from cruise altitude	20 seconds
Total Flight time	inutes

Table 4. Summary of thrust requirements

Flight Mode	Thrust Requirement (g)
Takeoff	96
Cruise, vertical component	20
Cruise, horizontal component	130
Hover	20

Table 5. Envelope Shapes

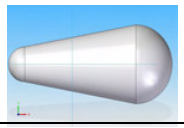
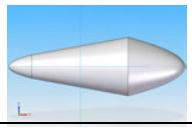
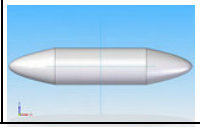
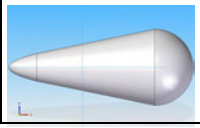
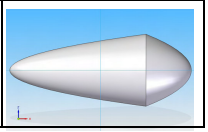
Concept	Tapered design with Hemisphere End	Tapered design with Elliptical End	Symmetrical design with Elliptical End	Hemisphere Front with Elliptical End	Different Elliptical Front End
Shape					

Table 6.Aerodynamic analysis of initial envelope shapes

Concept	Tapered design with Hemisphere End	Tapered design with Elliptical End	Symmetricald esign with Elliptical End	Hemisphere Front with Elliptical End	Different Elliptical Front End
Frontal Area Rank	5	2	1	4	3
Streamlined Profile Rank	4	1	5	3	2

Table 7. Surface Area to Volume Ratio

Concept	Tapered design with Hemisphere End	Tapered design with Elliptical End	Symmetrical design with Elliptical End	Hemisphere Front with Elliptical End	Different Elliptical Front End
Surface Area to volume Ratio	6.5	5.8	4.5	3.9	3.4

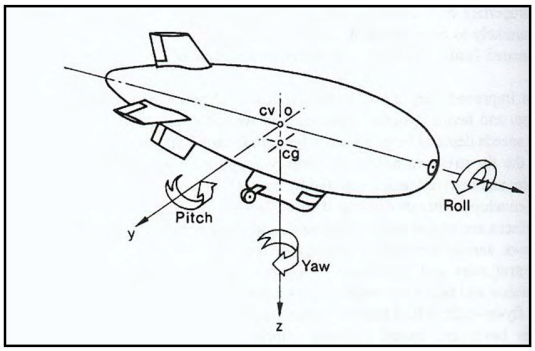


Figure 1 - The moments of an airship in flight

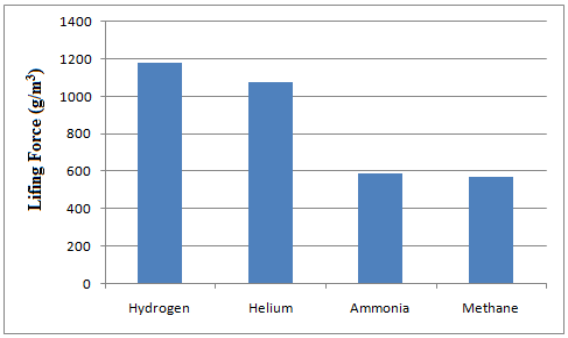


Figure 2 - Comparison of lifting force of gases

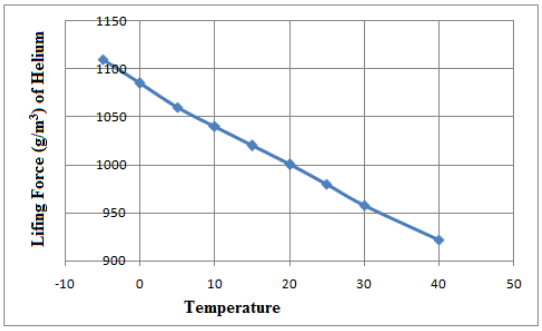


Figure 3 - Effect of temperature on lifting force

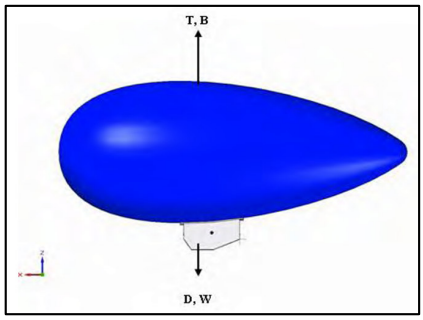


Figure 4 - Free body diagram of forces during takeoff

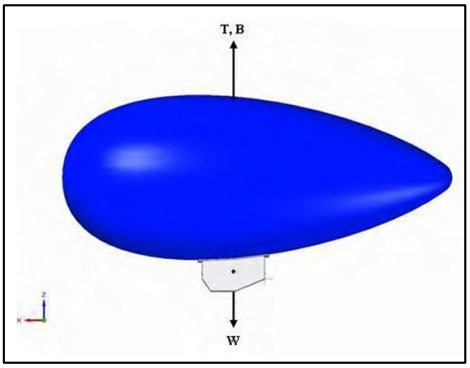


Figure 5 - Free Body diagram of forces during hover

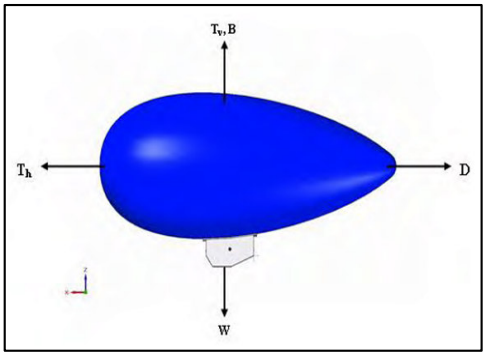


Figure 6 - Free body diagram of forces during cruise

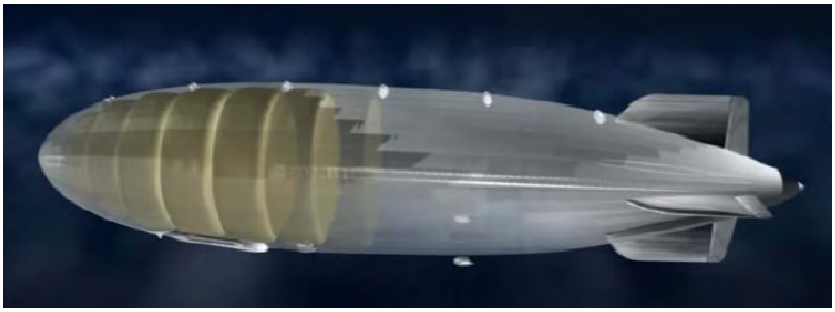


Figure 7 - Bladders in a rigid airship

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RESEARCH ARTICLE

Seasonal Impact on Gum Production of Three Plant Species from Tropical Forest of Sambalpur District, Odisha, India

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ABSTRACT

Plant gum is a major NTFP in natural forests, it has a significant role in commercial as well as in medicinal industry. Millions of tribal people earn their livelihood from collection and marketing of such plant gums. Odisha is a rich in vegetation of gum yielding plants like, *Sterculia urens* Roxb., *Acacia nilotica* (L.), *Anogeissus latifolia* (DC.) Bedd. *Azadirachta indica* A. Juss., *Lannea coromandalica* (Houtt) Merr., *Boswellia serrata* Roxb. Ex Coleb., *Shorea robusta* Gaertn.f., *Buchanania lanzan* Spreng. and *Aegle marmelos*. In this paper attempts have been made to find out a relationship between the seasonal condition and gum producing capacity of three different plant species i.e. Sterculia urens, *Boswellia serrata* and *Anogeissus latifolia*. The results indicate that the least production of gum has been found in the month of October (6.47 gin *Sterculia urens*, 1.23g in *Boswellia serrata* and 5.32gin *Anogeissus latifolia*) whereas production of gums in those plants reached in its maximum value in the month of June (14.97g In Sterculia urens, 4.4g in *Boswellia serrata* and 12.1g in *Anogeissus latifolia*).

Keywords: NTFP, gum tapping, exudation, seasonal impact, Water stress`

INTRODUCTION

India is one of the 17 mega biodiversity centers of the planet earth having a wealth of forest resources. The variation in soil quality, climate and topology across the country provides a suitable habitat for varieties of plant species and other life forms. It is estimated that the overall forest cover of India is 7,12,249 sq km. which is near about 21.67% of the total geographical area of the country[1], [2]. Apart from providing other ecosystem services (like regulating the climate, nutrient cycling etc.), the forest provides subsistence to a large section of the population of our country. Millions of tribal people earn their livelihood from collection and marketing of Non-Timber Forest Products (NTFPs).

Particularly in developing countries like India, gums and resins provide a significant proportion of NTFPs. Collections of gums and resins provide livelihoods to millions of Indian people living in or around forests.

Gums and resins are basically plant exudations that result partly from natural phenomena and partly by injury to the by insects, animal or human being. Gums and resins are generally exuded by plants in liquid form and on exposure to the environment it gets dry into translucent tears, and remain attached to the bark of the stem or branch [3]. These gums are otherwise known as tree exudates. These exudates (gums) have a historical background of about 5000 years, these are the composition of long chains of polysaccharides having high molecular weight, these polysaccharides are mainly composed of monosaccharide like, uronic acid and some protein and fibers [4].

A large number of gum and resin yielding plants are available in Indian forests, most remarkable among of them are plants *Sterculia urens* Roxb., *Acacia nilotica* (L.), *Anogeissus latifolia* (DC.) Bedd. *Azadirachta indica* A. Juss., *Lannea coromandalica* (Houtt) Merr., *Boswellia serrata* Roxb. Ex Coleb., *Shorea robusta* Gaertn.f., *Buchanania lanzan* Spreng. and *Aegle marmelos*(L.) Corr. [5]. Out of these *Sterculia urens, Boswellia serrata* and *Anogeissus latifolia are* some of the major gum-yielding plant species commonly found in the forest patches of Sambalpur district[3], [6]. Gum of these three plants have a lot of commercial uses in different industrial markets like paper, textile, petroleum and gas industries [7]. In addition to their commercial uses these gums are also used in pharmaceutical sectors. The different physical factors like temperature, humidity, sunshine, moisture, water stress and nutrient availability etc. influence the growth and metabolism of plants seasonally, also influence the production of gums in different seasons.

Coppen et al.1995 through their study have concluded that lower temperature normally leads to a depression in resin yield in pinus plants [8]. Study made by Rodrigues et al. (2009) on pinusplant also support Coppen's statement as they have shown that spring and summer influence more production of resin than winter [9]. Ballal et al. 2008 while studying on the effect of temperature on gummosis on *Acacia senegal*, have reported that high temperature during tapping period is conducive to high gum production while low temperature leads to sealing off of the gum exudation points as a result there is no gum yield [10]. Fahn et al. 1979has done a similar study on seasonal effect on wounding and gum production in Cedrus plant and they have concluded that wounding from April to October, when the temperature was higher and cambium was active, resulted in larger sized ducts formation than the ducts formed by wounding in other months [11].This could be the reason for high gum production during the hot season.

Few studies have also been made in India to see the effect of different season on gum production. The best season for optimum gum and resin collection is March to June when temperature is maximum in the environment [12], high ambient temperature may accelerate gum oozing which also been reported earlier by Bhatt et al 1987 [13]. Trees of Tropical region may show higher gum yielding potentiality. A systematic investigation on the production of gum in different gum yielding plant species in different seasons has become a basic need which will help to make proper planning for development of the best commercial tapping schedule.

MATERIALS AND METHODOLOGY

Study site

Present study has been done in thecommon forest patches of Sambalpur district, Odisha. viz. "Lakhmidungri", "Daridungri" and "Chandlidungri"in the Kamgamforest range, Sambalpur south forest division, Sambalpur. Lakhmidungri(21^0 28′ 24.02″ N to 21^0 45′28.78″N and 83^0 52′ 02.12″ E to 83^0 77′ 45.23″E)with an area covering of 333.34 hectare (average altitude 170 m),Daridungri($22^025'48.66''$ N to $22^039'56.32''$N and $83^052'54.07''$ E to $83^067'55.01''$E)with an area covering 30.12 hectare (average altitude55m) and Chandlidugri ($21^029'15.78''$N to $21^055'43.22''$N and $83^055'44.63''$E to $83^069'54.31''$E)with an area of 415.27 hectare (average altitude220 m) are tropical dry deciduous forestswith tropical monsoonic climate .

METHODOLOGY

In traditional method of tapping wounds were made by axe or some homemade instruments which causes undefined wound formation due to uncontrolled pressure on the stem of the plants and that leads to irreversible damage to the plants [14]. Therefore, in the present experiment a standard tapping tool chisel (2cm. & 5 cm. widths) and hammer (250 g.) were used to form definite size (10cm X 10 cm) of wound by exerting controlled pressure [15]. To ascertain the seasonal impact on gum production, gum trapping was done on the selected plant species during the dry seasons (except the rainy season i,e July, August and September) at monthly interval basis by following the method of Fahn et al. (1979) and Ballal et al. (2009). The gum thus produced from the standard wound at standard height at the right direction in different months were collected, dried and weighed to find out the effect of seasonal variation on gum production [11], [16].

RESULTS

The gum production recorded in different months of the year from all the three different plants i.e. *Sterculia urens*, *Boswellia serrata* and *Anogeissus latifolia* at a previously standardized height (150 cm. from the ground) from standard wound size (10X10 cm.) revealed that the gum can be harvested throughout the year, though at differential amount except the rainy months of July, August and September of a year. Table1 depicts the effect of season on the yield of gum from *Sterculia urens* , *Boswellia serrata* and *Anogeissus latifolia*. Results shows that Sterculia urens has more gum production potentiality followed by *Anogeissus latifolia* throughout the year.The gum production in all thethree plants from the wound was found to increase linearly from January to June (Fig. 1). June inwards in the month of July August and September the gum production was almost nil. Thereafter from the months October onwards the gum production exhibited an increasing trend in all the three plant species. The highest amount of gum produced in all the three species was found in the month of June i.e.14.97g In *Sterculia urens*, 4.4g in *Boswellia serrata* and 12.1g in *Anogeissus latifolia*.

DISCUSSION

The gum production in different months of the year varied significantly in all the three species of plants. In all the species the gum production went on increasing from January -June and it reached its maximum value in June. Thereafter in July-September which is locally the rainy season there was almost no measurable quantity of gum production and whatever minimal amount was produced those were washed away by rain water. After the rainy season (October-December) a slight increase in gum production was observed. The highest amount of gum production during May and June months of the year could be due to the un-conducive environmental conditions (like high temperature, less humidity and water stress) prevailing during this month which favours high amount of gum production. Coppen and Hone (1995), Pio and Valente (1998) and Brito et al (1982) have also reported that lower temperature normally lead to a depression in resin and gum production from plants [8], [17], [18]. The influence of photoperiod cannot be disregarded since ethylene (an inducer of gum production) biosynthesis is induced by light and is circadianly regulated [19].

Transcripts of genes encoding some terpene synthesis have also been shown to follow a weak diurnal oscillation that is under the control of circadian clock [20]. The findings of this study that high temperature at tapping time is conducive to high gum production while a low temperature seems to seal off the gum exudation points resulting in low yield of gum, is in conformity with the report made by IIED and IES (1989)[21].Dione and Vassal(1998) have also reported that peak gum production is apparently stimulated by the onset of drought condition i.e. after in rainy season and air temperature rises[22]. Another reason of high amount of gum production during drier months of the year is due to the presence of higher level of reserve metabolites in plant tissue [23]. This seems to explain why greater exudated yields are obtained during the dry months of May-June than during any other months. Fahn et al.

(1979) have further reported that during the hot and dry months of the year, the cambium remains active and more gum ducts are formed leading to increase in gum production [11]. The reverse happens during the cooler and wet months of the year.

CONCLUSION

From the above investigation on the study of sessional variation of gum yields on three tree species viz.*Sterculia urens, Boswellia serrata* and *Anogeissus latifolia,* it was observed that there is a significant variation on gum yields among the three plants with respect to different seasons. It can be concluded that*Sterculia urens*has significantly more gum yielding potential followed by *Anogeissus latifolia*. while Seasonal variation is concernthat May and June is comparatively best season when the gum yielding is maximum in all the three plants.

ACKNOWLEDGMENT

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Table-1: Effect of season on the yield of gum from *Sterculia urens* ,*Boswellia serrata* and *Anogeissus latifolia*

Months	*Sterculia urens* gum (g/wound)	*Boswellia serrata* gum (g/wound)	*Anogeissus latifolia* gum (g/wound)
January	8.34±0.98	2.32±0.55	6.85±1.01
February	8.82±1.21	2.45±0.48	7.32±1.23
March	9.01±1.14	2.65±0.57	8.09±1.41
April	11.31±1.32	3.2±0.91	9.11±1.92
May	13.99±1.4	3.43±0.89	11.07±1.24
June	14.97±1.27	4.4±0.59	12.1±1.41
July	0	0	0
August	0	0	0
September	0	0	0
October	6.47±0.99	1.23±0.45	5.32±0.58
November	7.66±1.47	1.87±0.51	6.02±0.88
December	8.1±1.39	2.22±0.49	6.6±0.78

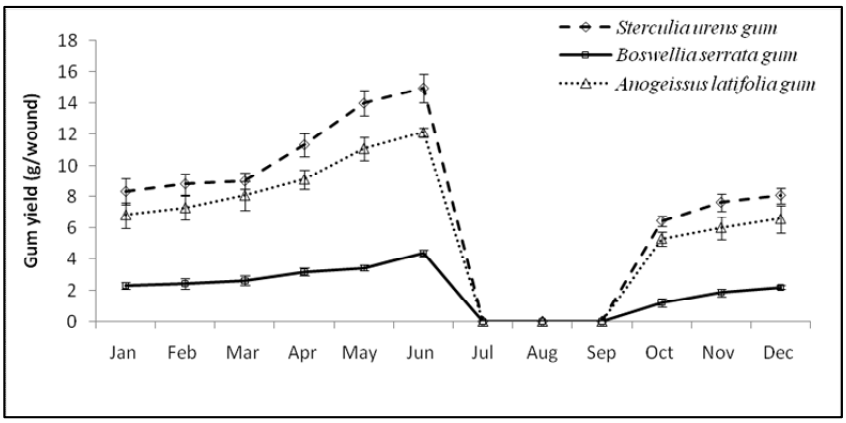

Figure-1: Effect of season on the yield of gum from *Sterculia urens* , *Boswellia serrata* and *Anogeissus latifolia*

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RESEARCH ARTICLE

The Distribution Pattern of Foliose Lichen in Different Forest Region of Keonjhar District, Odisha, India

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ABSTRACT

This is the new survey report in Keonjhar district of Odisha. In consonance with the survey report, we are found in 13 number of species of foliose lichens pertain to 8 genera and 3 families at the place of Salandi, Kanjipani and Champua. The three families are Physciaceae, Parmeliaceae and Arthoniaceae. In these three areas of Keonjhar district, the most dominate tree is *Shorea robusta* (Sal tree) which is much more flourishing foliose lichen and other trees are also carry on foliose lichens correspondingly trees are *Bombax coiba*, *Dalbergia sisso*, *Saraea asoca* and *Delonix rejia*. Above the 13 number of species of foliose lichens are maturing on tree bark. This is the preliminary survey report. Further we are study, we will be achieve more numbers of different types of lichen i.e. Crustore, foliose and fruticose lichens.

Keywords: Foliose Lichen, Kanjipani, Champua, Salandi (Hadgarh sanctuary) Keonjhar district, Odisha, India.

INTRODUCTION

Lichens are the successful symbiotic interact small plant or organisms that have consist of the fungi (mycobiont) in abxial position and algae (phycobiont)in adxical position [1]. Generally we are known lichens are divided is 3 major groups such groups are Crustose, foliose and Fruticose. Foliose lichens are leaf like structure and adhere to their substrate loosely. Crustore lichens are looks like crust and embedded in their substrate. It has no lower attached. In earth, this type of lichens is found in 75%. Fruticose lichens have no distinct top and bottom and its thalli may be upright, shrubby [2].

Accordingly foliose lichens are one of another variety of lichens. Foliose lichens are complex organisms which arise from the symbiotic relationship between fungi and algae. In this lichens lifespan is between 30 to 60 years [3]. Lichens contain a main part of body called the thallus which is composed of hyphae, cortex and medulla. The cortex contains the photosynthetic cells, medulla is gas exchange. Foliose lichens attach to surface by hyphae in the lower cortex with root like structures called rhizines. In environmental case, lichen also major role. Lichen provides a food source for many animals that animals are dears, goats and caribou and also building for bird nests. Some species are used for medicine and also used as indicator of atmospheric. In the case pollution, these lichens are sensitive to sulphur dioxide which is a by-product of atmospheric pollution. Sulphur dioxide reaction with chlorophyll in lichen which is produce in phaeophytin and magnesium ions [4]. In the case of reproduction, these lichens are show two types of reproduction system i.e. sexually and asexually. The reproduction both requires fungi and algae. Reproduction of lichens, the fungal partner must be produce millions of germinating spores which fuse to zygote that found a compatible photobiont. This photobiont fuse with the zygote and create lichen. The fungal partner is ascomytes with spores called ascomata. The lichen of fruiting bodies make up one of two shapes which looks like disk or cup shaped and produce their upper surface which shaped flasks like that is spore producing layer with a hole at the top. Foliose lichen use cylindrical finger like protuberances from the upper cortex which is algal and fungal tissue. They are easily breakdown and spread by wind and they will relocate and propagate forming new lichen [5].

Lichens are world wise distribution. In India is a subcontinent of Asia, it is also rich in lichens which is mostly found in 8 lichenogeographic region such regions are Western Himalaya, Eastern Himalaya and North east India, Western Dry Region, Gangatic plain, Central India, Western Ghat, Western Ghat and Deccan Plateau, Andaman and Nicobar Islands. In world wise reported 20000 species of lichens found and the subcontinent of India also carry 2450 species of lichens and more than 2300 species of lichens only Indian possesses [6].

The mega diversity of India which is more than 10% of total world lichen species hold about 2303 species belong to 305 genera and 74 families widely distributed in tropical, sub-tropical, temperate and alpine zone of India [6].

Odisha is state of India which is located within the latitudes $17^0$78/N &$22^0$73/ and longitudes $81^0$37/&$87^0$53/. The state of Odisha is bounded by West Bengal on the North east, north side is Jharkhand, Chhattisgarh is west side, Andhra Pradesh is south side and the east side is Bay of Bengal. The costal line of Odisha about 450kms and the total area of Odisha are about 1, 55, 707km2.The state of Odisha which is contain 252 speciese of lichens belongs to 81 genera and 35 family that is 49 species of Graphidaceae, 21 species of Arthoniaceae, 19 species of Pyrenulaceae, Parmeliaceae (18), Trypetheliaceae (17), Physciaceae (15), Teloschistaceae (14), Lecanoraceae (13), Pertusariaceae (12), Ramalinaceae (11), Caliciaceae (11), Thelotremataceae (9) and Lecidiaceae (4). The Graphidaceae family of genus Graphis which ig dominat 27 species in the stat of Odisha followed by Pyrenula (16), Caloplaca (14), Pertusaria (12), Lecanora (10), Parmotrema (9), Cryptothecia (9) and Pyxine (6). The most of lichens are found in Mayurbhanj district which is 141 species and followed by Jharsuguda 31 species,Ganjam 21 species, Gajapati (7), Dhenkanal (5), Koraput (3), Khordha (3), Puri (1), Sambalpur (1) and Sundergarh (1). Most of 20 districts are complitely uninvestigated for lichens. Only 10 districts are found in 252 species of lichens [7]. Some of species of lichens are identified by Keonjhar district. The briefly describe in foliose lichen in different host plant at Keonjhar district.

MATERIALS AND METHODS

STUDAY AREA

Keonjhar district is an administrative district of Odisha. It has three sub- divisions i.e. Anandapur, Champua and Keonjhar. Keonjhar district is occupied area 8240km^2 and longitude $86^0$21/ E & latitude $21^0$59/ N. Keonjhar district maximum temperature is 38^0C to 43.3^0C and minimum temperature is 1^0C to 7^0C. According to weather forecast department, in November & December minimum temperature is 1^0C. Keonjhar district annual rain fall is 1910.1 mm

recorded. Among the Keonjhar district, we are selected three sides- Salandi (Hadgarh sanctuary), Kanjipani and Champua then go to these three areas and watch it and study clement condition and other environmental study with site or area location. Salandi forest is situated in Anandapur, district of Keonjhar, Odisha. It is located in latitude 21.289335^{0}N and in longitude 86.320443^{0}E. Hadagarh Wildlife Sanctuary is dense forest which is constituted in Sal trees i.e. the dominate trees of this Sanctuary which is established in 1978 and it's covered in 191.6 sq. km. Salandi forest is linked to Similipal Tiger Reserve and with Kuladiha Wildlife [8]. Champua is situated in sub division of Champua which is district of Keonjhar, Odisha. Its Latitude is 22.0800N and longitude is 85.6700E and in this area clement is moderate and it has an average elevation of 346 metres. Kanjipani Ghati is situated in Keonjhar district. This area spreading about 20km along NH- 49, from Kanjipani to Jagamohanpur and about 8km along Telkoi road i.e. Kanjipani to Panassanasa. Kanjipani Ghati is located on longitude 85.4608^0 E and latitude 21.4705^{0}N. In this area temperature is 0^{0}C in winter and rainy season but summer season temperature is about 25^{0}C to 30^{0}C. So, in this area is less pollution and lichens are well growth in this area. Kanjipani also carry a vast area of flora and fauna and with Huge Wildlife reserves.

COLLECTION, PRESERVATION AND IDENTIFICATION

The lichens are divided two groups i.e. micro and macro lichens. So, commonly visible micro and macro lichens for our naked eyes. First watch the micro and micro lichens then start digging it by the equipment of a long sharp fat edged chisel (1 to 2 inch.) and a hammer (1 to 2kg weight) with GPS that is use for location and pan and paper due to wright some information i.e. name of area, note of location and note of trees name with date and also take camera for click photos for macro and micro lichens with trees. In this way collected lichens then start next process that process is preservation. So, preservation processes are first collected lichens or samples are put out the carry bag then this samples dry by heat air or sun light with in 24hours then pressed by herbarium pressure due to simples are not bend, within 2 to 3 days. After 2-3days, the samples are ready to identification, so, 1st make some packet that colour is white or brown, then put on the specimen or samples or lichens and wright down some information that is name of area, date etc. After all this work is complete then starts next process that is identification. Lichens are identified by morphological and anatomy of thallus structure and mode of reproduction [2] by using available of standard keys[9, 10, 11, 12, and 13]. One method used for identification in lichens consists of some spot test. It is based on three chemical tests that may or may not yield a colour change when applied to lichen. Now a day thin layer chromatography (TLC) is the most widely used method for identification of lichens. Then extracts of the unknown lichens are spotted on a TLC plate. Picture 2 a,b & c representing the growth of foliose lichens in different host i.e. tree substratum.

RESULT AND DISCUSSION

According to survey report, we are found in 13 species of foliose lichens which belongs to 8 genera; there are found in various parts in Keonjhar (Salandi, Kanjipani and Champua). This survey report is based open the foliose lichen in diversity host. These are level in following table.

Serial Number	Name of the tree	Family	Lichens name	Type of lichens	Growth area
1	*Delonix rejia*	PARMELIACEAE	*Parmotrema reticulatum*	Foliose	Champua
2	*Shorea robusta*	ARTHONIACEAE	*Dirinaria applanata* var. applanata D.D. Awasthi.	Foliose	Salandi(Hadgarh sanctuary)
3	*Shorea robusta*	ARTHONIACEAE	*Dirinaria consimilis* (Stirt) D.D. Awasthi	Foliose	Salandi(Hadgarh sanctuary)
4	*Shorea robusta*	PARMELIACEAE	*Bulbothrix isidiza* (Nyl.) Hale	Foliose	Kanjipani

5	*Shorea robusta*	PARMELIACEAE	*Myelochroa xantholepis* (Mant. & Bosch.) Elix	Foliose	Kanjipani
6	*Shorea robusta*	PARMELIACEAE	*Parmotrema andium* (Mull. Arg.) Hale	Foliose	Champua
7	*Shorea robusta*	PARMELIACEAE	*Parmotrema ravum* (Krog & Swinscow) Serus	Foliose	Champua
8	*Saraca asoca*	PARMELIACEAE	*Parmotrema tinctctorum* (Despr. ex. Nyl.) Hale	Foliose	Champua
9	*Dalbergia sissoo*	PHYSCIACEAE	*Pyxine coccifera* (Fee) Nyl.	Foliose	Salandi(Hadgarh sanctuary)
10	*Shorea robusta*	PHYSCIACEAE	*Heterdermia pseudospeciosa* (Kurok.) Culb	Foliose	Kanjipani
11	*Bombax ceiba*	PHYSCIACEAE	*Heterdermia obscurata* (Nyl.) Trevis	Foliose	Kanjipani
12	*Shorea robusta*	PHYSCIACEAE	*Heterdermia diademata* (Taylor) D.D. Awasthi.	Foliose	Kanjipani
13	*Bombax ceiba*	PHYSCIACEAE	*Heterdermia albidoflava* (Kurok.) D.D. Awasthi	Foliose	Kanjipani

(**The above table shows the categories of host plant in grow family of foliose lichens that is Physciaceae which is found in more number and also Heterdermia species of lichens growth in more number in these three areas.)**

Three families are Arthoniaceae, Parmeliaceae, and Physciaceae. This foliose lichen is growth in different site of Keonjhar district that sites are Salandi, Kanjipani and Champua. We are observed, the Sal trees are dominating tree in Keonjhar district which is suitable host body for lichens growth and also observed Kajipani is one most wonderful place which contains more number of foliose lichens i.e. 6 numbers of foliose lichens then Champua contain 4 numbers of foliose lichen and Salandi contain 3 numbers of foliose lichens. In these 3 sites, the 13 numbers of foliose lichens are *Dirinaria applanata, Dirinaria consimilis, Anisomeridium terminatum, Bulbothrix isidiza, Parmotrema tinctctorum, Parmotrema andium, Pyxine coccifera, Heterdermia albidoflava, Heterdermia pseudospeciosa, Heterdermia obscurata* and *Heterdermia diademata*.

In the above graph (Fig-3) foliose lichens grow on this trees such trees are*Shorea robusta, Bombax ceiba, Dalbergia sissoo, Saraca ascoa,* and *Delonix rejia*. The relationship between lichen and tree is commensalism that is one organism benefits form the association and another is neither positively nor affected. So that lichen is use tree as structural roosts. Lichen is a unique organism that a symbiotic relationship between algae and fungus. We are known fungus are grow on trees at that time fungus are collect moisture that is helpful for the algae. Then the algae can produce food by the help of sun light which feeds the fungus.

Form above pic-chart (Fig- 4) shows that the different geo-graphical region of Keonjhar District (Salandi, Kanjipani and Champua). Kanjipani is suitable place for growing more number of foliose lichen (46%) carry on because this area has less pollution and suitable climate condition for growth in lichens. Then Champua also carry on 31% of foliose lichens as well as Salandi (Hadgarh sanctuary), also carry on 23% of foliose lichens. Form above pic-chart (Fig- 5) shows that, the distribution of lichen family. The Parmeliaceae (48%) family have highly distributed in foliose lichen then Physciaceae (39%) which is moderate distributed and Arthoniaceae (15%) which is quit listed number of distribution in Keonjhar district.

CONCLUSION

From above preliminary study, we conclude that 13 numbers of foliose lichen species are distributed into Salandi, Kanjipani and Champua in the Keonjhar district. These lichens drivers from tree bark that trees are *Shorea robusta, Bombax ceiba, Dalbergia sissoo, Saraca ascoa,* and *Delonix rejia.*

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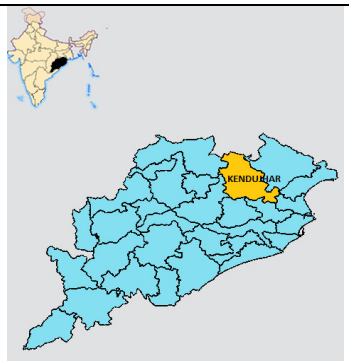

Fig.1. Keonjhar district map, Odisha, India

Fig.2 a

Fig.2 b

Fig.2 c

Fig 2 a,b & c representing the growth of foliose lichens in different host i.e. tree substratum.

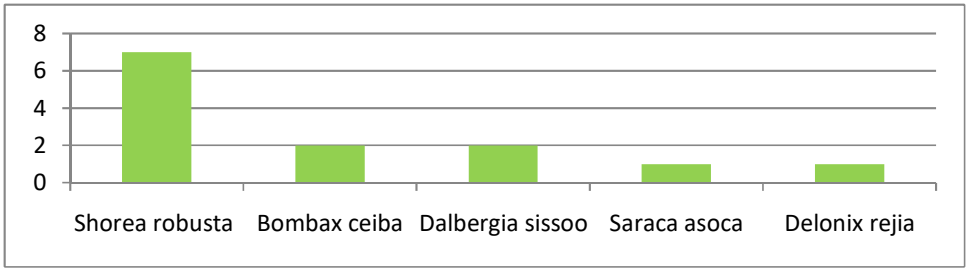

Fig.3: Growth of foliose lichen in different tree species in Keonjhar district)

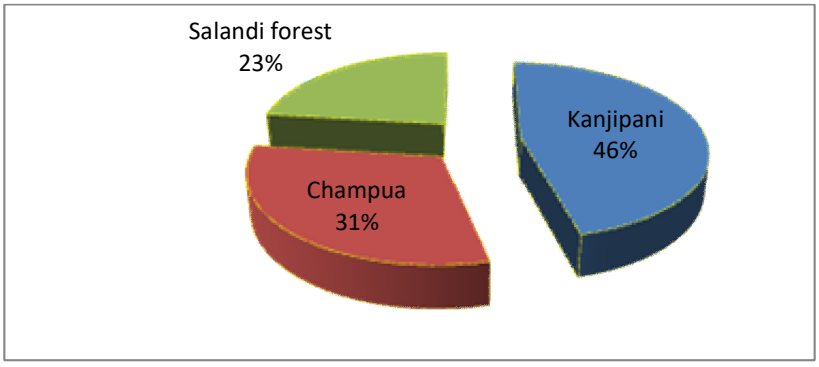

Fig.4 Growth of foliose lichen in different forest area in Keonjhar district

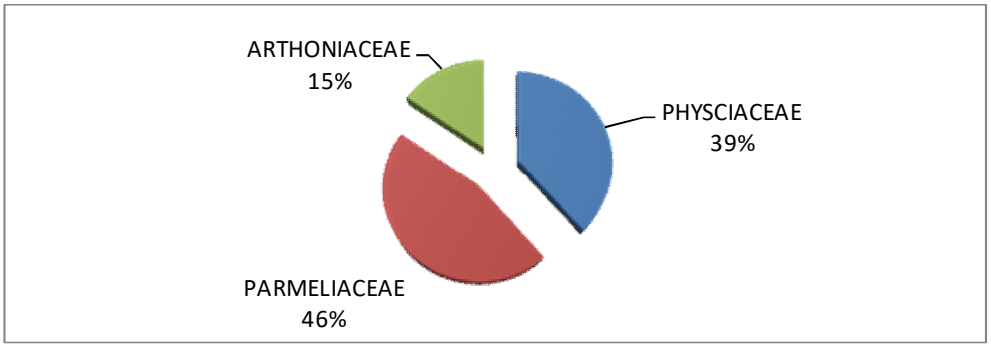

Fig.5. Family wise distribution of foliose lichens

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RESEARCH ARTICLE

Design & Performance Comparison of 8*8 Multiplier Circuit using Modified Gate Diffusion Input Adder Cell

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ABSTRACT

In this paper design and simulation has been carried out for 8*8 multiplier circuits using the Modified Gate Diffusion Input (MGDI) based adder cellusing Digital Schematic (DSCH3) CAD tools and their simulations are generated by Micro wind 3 CAD tool. Further the performance assessment comparison of multipliers were made.Adder has been known to be the basic building block of all arithmetic operations, thus the focus is also to optimize the adder circuit that can be implemented in different multiplier algorithms and to compare their results in terms of area, operating speed, power consumption and transistor count.

Keywords- MGDI modified GATE diffusion technique, CAD-computer aided design

INTRODUCTION

In VLSI design configuration, the rapid development of convenient electronic gadgetwith limited power and area ha s opened up a wide range of chances and difficulties for less power and small circuit design.Multiplication is a key function in arithmetic logic operation, imageprocessingandinDSPalgorithms.Andso it is desirable to make low power, highspeed multiplier circuits for these operations. This multiplication often uses the adder circuits. Various types of logic are suggested for high speed and less power consumption, and every sort of logic has its own advantage and disadvantage in terms of power consumption and speed. MGDI is defined as one of the alternative logics that can boost the efficiency of the circuits .using a single pair of transistors (one NMOS and one PMOS),a

wide range of logic functions can be realized in MGDI technique. This leads to reduced power and area compared with current CMOS technology.[1].Input 'G'is the PMOS and NMOS shorted gate terminal,'N' is obtained from the NMOS source terminal and 'P' is obtained from pmos. Body terminal of PMOSis connected to V_{dd} and NMO Sis connected to Gnd respectively. Table 1 shows the various functions that can be obtained using this MGDI cell. In fact, these functionshave been mentioned in table 1 require 6 to 12 transistors to be implemented using CMOS, But with one pair of transistors, can also be implemented.Table II reveals comparison of the transistor numbers for different functions [2].

In the present paper, a new adder cell is proposed to implementan8 ⊙ 8 bit multiplier circuit. Our proposed cell is designed using a combination of both the MCIT and the Shannon technique. This paper describes the design of an adder cell for digital applications, such as those used in DSP algorithms and cryptography. The proposed adder cell is applied to implement three different types of 8 ⊙ 8 bit multiplier circuits: namely a Braun array multiplier, a CSA array multiplier and a Baugh–Wooley array multiplier. These multipliers are designed using CAD tools such as DSCH2 for logic design and Microwind 3 for the layout design and timing simulation. In the present paper, a new adder cell is proposed to implementan8 ⊙ 8 bit multiplier circuit. Our proposed cell is designed using a combination of both the MCIT and the Shannon technique. This paper describes the design of an adder cell for digital applications, such as those used in DSP algorithms and cryptography. The proposed adder cell is applied to implement three different types of 8 ⊙ 8 bit multiplier circuits: namely a Braun array multiplier, a CSA array multiplier and a Baugh–Wooley array multiplier.

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METHODOLOGY

Design and Architecture

The following multipliers are designed in 0.35 μm as well as 0.25 μm design sizes using the DSCH2 and Microwind VLSI CAD tools:

1.Carry save array multiplier .

2. Braun array multiplier.

3.Vedic multiplier

Carry Save Array Multiplier

Carry save array multiplier is suitable for both signed and unsigned numbers. To aggregate the partial product it uses a variety of carry-save adders. The multiplier utilizes a carry-propagate adder for the finished product. This decreases the basic path delay for the multiplier, as the carry-save adders pass the carry to the next degree of adders rather than nearby ones. Figure 2.4 shows the 4 * 4 carry save array Multiplier architecture[10]. Consider the two binary numbers to be multiplied by X and Y. Where X is the multiplicand, and Y a multiplier.

$X=x_{n-1}x_{n-2}x_{n-3}\ldots\ldots x_1x_0$

$Y=y_{n-1}y_{n-2}y_{n-3}\ldots\ldots..y_1y_0$

$P(product)=p_{2n-1}p_{2n-2}p_{2n-3}\ldots..p_1p_0$

Half adder, full adder and the AND Gate blocks have been in use incarry save multiplier architecture.

Braun array multiplier

Braun Array is a simple parallel multiplier, consisting of AND gates and carrying save adders as shown in the figure below.For an N*N Braun array multiplier, the number of AND gate required is N^2 and no of carray save adder required is N*(N-1).Partial products are created in parallel using the AND gates. Partial products are added with the sum of the previously generated carry save adder output using adders in rows. The final phase output is obtained using the ripple carry adder [9]. This multiplier preferred for positive operands.Figure 4 liststhe Braun algorithm for non-signed binary multiplication

Vedic multiplier

Vedic mathematics helps with less delay in quick calculation, because in Vedic mathematics the algorithms are based on human mind interpretation. There are various multiplicationmethods are there in Vedic mathematics. Among them the Urdhvatiryagbhyam, as a basic rule for multiplication, it applies analogously to all forms of multiplication.This boosts speed and area of multiplication by significantly.

Implementation: Adder design

Half Adder designing using MGDI

The half-adder circuit takes two inputs as augend and addend bit, and produces the output as a sum and carry. The sum output and the carry output shall be expressed as SUM = A⊕B and CARRY = A.B.The figure below shows half-adder design with MGDI technique.

Full Adder Designing using MGDI

The full adder is a combination logic circuit which uses 3 bits as inputs to add and produce the sum(s) and carry(c) as output along with a previously produced carry.The proposed adder cell using modified gate diffuse technique MGDI , with 8 no of transistor is shown in below figure.

Multiplier design

Proposed adder cell can be applied for making multiplier circuits.Half adder and full adder circuit were designed at first and the output is checked.Afterthat library module for these cell was made which isdirectly used in the design of multiplier circuits.Fig.9 demonstrates the Carry save array multiplier being implemented in DSCH3 and the output is displayed on the led display.

Vedic multiplier

With the MGDI adder cell and 4*4 multiplier as building block,8*8 multiplier is designed in DCH3.

Comparative Analysis of Multiplier Circuit

Three types of multiplier circuits have been designed and evaluated using digital schematic DCH3 VLSI CAD tool and the performance evaluation are done in Microwind3 .The parameter like power dissipation, critical path delay and area occupancy is obtained for 0.12um and0.32um feature size technology. The simulated result for the 8*8 multiplier circuit is compared in the given table 2&3.

CONCLUSION

The 8*8different multiplier algorithms such as Carry Save Array, Braun Array and Vedic multiplier with MGDI technique in 120nm and 320 nm is designed using DCH3.for performance ,among them the Vedic multiplier gives the optimal results with regard to total chip area, power dissipation, delay and total transistor count .

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Table 1 displays the different functions which can be realized using MGDIcell[1]

N	P	G	OUT	Function
0	B	A	A'B	F1
0	1	A	A'+B	F2
1	B	A	A+B	OR
B	0	A	AB	AND
C	B	A	A'B+AC	MUX
0	1	A	A'	NOT

Table II :Comparison of transistor count for CMOS and MGDI technique

Logic function	CMOS(no of transistor)	MGDI(no of transistor)
F1	6	2
F2	6	2
OR	6	2
AND	6	2
MUX	12	2
NOT	2	2

Table -3 Performance comparison of multipliers in 0.12µm Technology

Multiplier	Pd(mw)	Transistor count	Delay (ps)
Braun Array (8*8)	29.487	116	308
CSA (8*8)	22.323	186	245
Vedic multiplier(8*8)	7.115	142	105

Table .4 Performance comparison of multipliers in0.35µm Technology

Multiplier	Pd(mw)	Transistor count	Delay (ps)
Braun Array (8*8)	17.487	116	502
CSA (8*8)	15.123	186	600

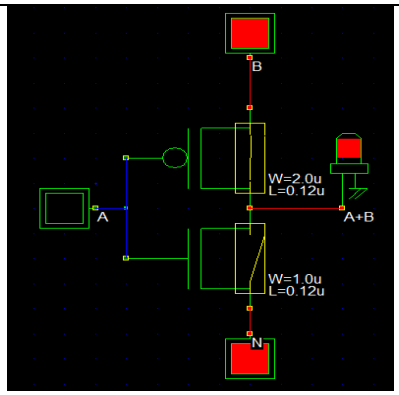


Fig: 1 Structure of MGDI cell

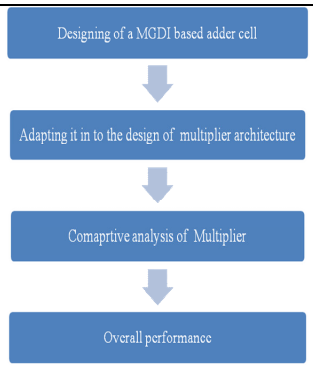


Fig. 2 Flowchart of Methodology

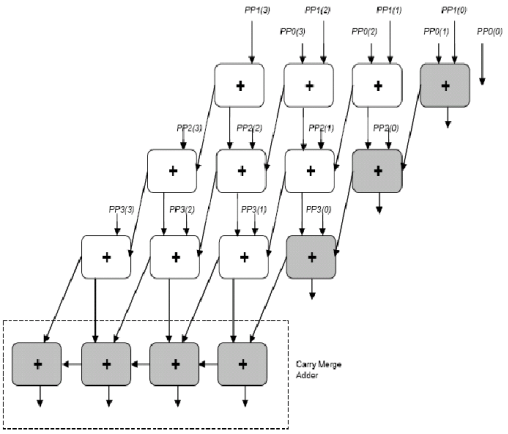


Fig .3 Carry save array multiplier

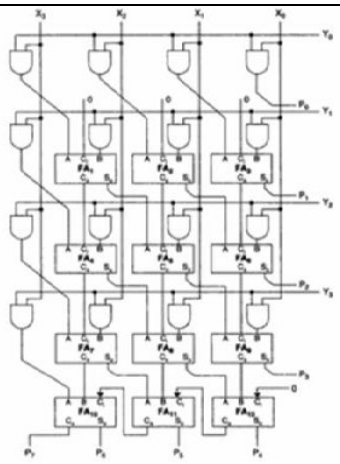
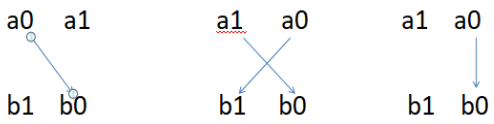


Fig .4 Braunarray multiplier



- s0=a0b0
- c1s1=a1b0+a0b1
- c2s2=c1+a1b1

Vedic Multiplication Method For 2bit Binary

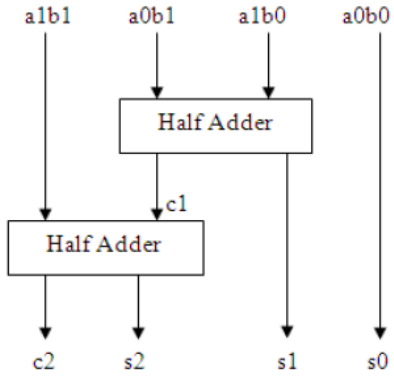


Fig .5 Architecture of 2*2 Vedic multiplier

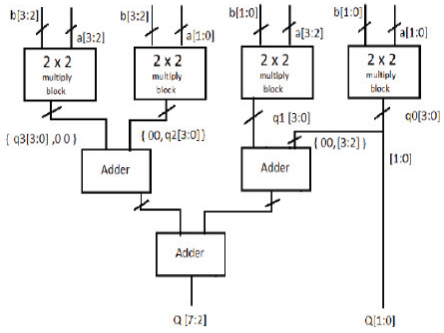


Fig. 6Architecture4*4 Vedic Multiplier

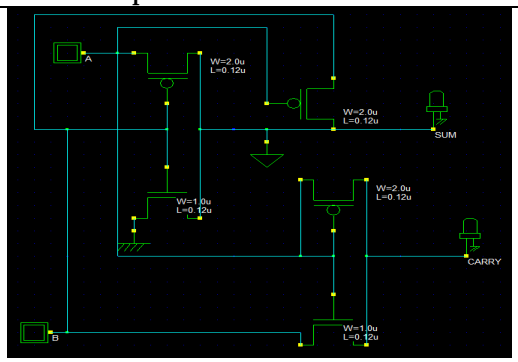


Fig .7 Architecture of half adder using MGDI

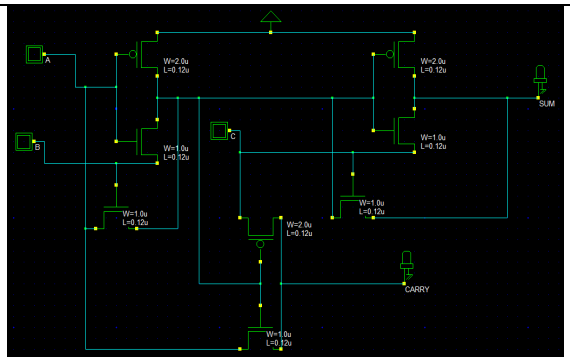


Fig -8 Full adder circuit using MGDI technique with 8 trasistor.

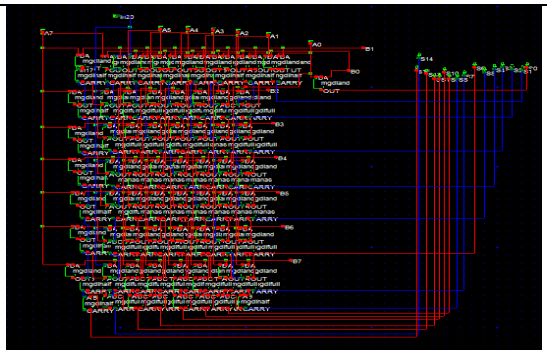


Fig-9 8*8 Bit Multiplier in CSA

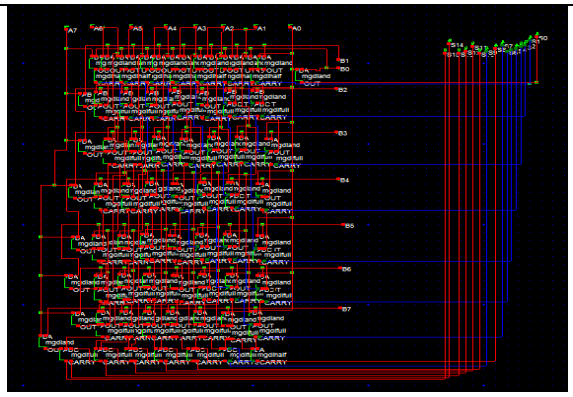


Fig-10 8*8 Bit Multiplier in Braun Array

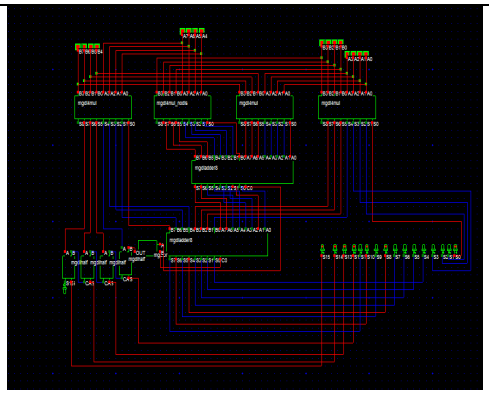


Fig-10 8*8 Bit Vedic Multiplier

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RESEARCH ARTICLE

Comparative Evalution of Egg Quality Characteristics of Indigenous Variety of *Gallus gallus domesticus*

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ABSTRACT

In this present investigation which was layout to examine the internal and external egg qualityattributes of indigenous chickens of five phenotypes. The study was carried out at Centurion University, poultry farm, in the Department of Zoology. The research drudge for a period of two months. Ten eggs of each phenotypes were collected randomly for the study. Fifty egg in total were possessed for the study. For determination of parameters instruments like digital electric balance, Micrometer screw gauge and Vernier calliper were made used. Egg width, albumin height and width significantly ($p<0.001$) differ among the phenotypes. A significant difference ($p<0.001$) differs in the egg width, albumin height and width. Except Haugh unit other egg quality attributes were significantly affected by the type phenotypes. SimilarlyVanaraja have the highest egg weight, egg volume, egg width and yolk weight. But in V_2 chabro have the lowest egg weight, egg volume, albumin length, albumin height, yolk length, yolk height. Red Cornish have the highest moisture content, while black rock have the highest protein content and Dhelem red have the higher lipid content than other indigenous species. Energetic value content more in V_2chabro and highest carbohydrates present in Red Cornish.So the objective of present study is to provide information about the comparative physicochemical characteristics of eggs of different layers which includes different strains of Gallusgallusdomesticus

Keywords: Phenotypes, egg quality, Vernier calliper, Digital electric balance, Sphaerometer**,** Screw gauge

INTRODUCTION

Eggs are highly accomplished food consisting vital source of fibres useful for maintaining human health. Eggs produce a unique and well balanced nutrient for all ages. The connotation of proteins in animals present in plentiful and equitable substances is considered for the human affluence with beneficial to mental and physical advancement

[1]. Between aforementioned such animal protein sources, the poultry animals have an important place for the meat and egg production. The productiveness and distinctive attributes of breeding eggs have an overall implication for the progression of flocks and for an economic breeding [2]. The nutritional composition of eggs of different species of birds may be similar in terms of nutritious composition. Nonetheless, facts about the egg quality traits and its application in food and other industry are restricted mainly to hen's eggs. The egg quality that influences its reliability to consumers are weight of egg, the quality of shell, the yolk and albumen index and most acceptable quality i.e., its freshness of eggs as well as its proximate composition [3-4]. Quality of the egg is the main price determining factor in table and hatching eggs. Chicken eggs have been very competently analysed for its external and internal qualities as well as its admixtures. Hence, this study presents a comparative analysis of the morphological structure and chemical constitution of eggs of chicken species which have economic as well as considerable nutritional value.

MATERIALS AND METHODS

The eggs of turkey and chicken used for this study analysis were assembled from the farm of Central Poultry Development Organisation (CPDO), Bhubaneswar. The eggs were assembled on the day of fling down in the month of November, 2018. During laying time, the chicken were 275 days old. The bird were nurtured under farm conditions on the chicken specialized dietary suitable for chickens.

Evaluation of egg quality

The external characteristics of egg like egg weight was measured in an analytical balance of Dhona – 200 (AB-204) after cleaning and parched with towel to remove contaminants from shell. The egg length and width were measured with a Vernier calliper in centimetre and egg shape index was obtained by the following formula.

$$\text{Shape index} = \frac{\text{Width of egg}}{\text{Length of egg}} \text{ x } 100$$

To examine the internal egg quality characteristics each egg samples were ruptured on a flat white title by taking precautions for not breaking the vitelline membranes which encloses the yolk. The parameters measured were as follows.

a) Yolk width was measured as the widest horizontal circumferences with a Vernier calliper in centimetres.
b) Yolk height was measured as the height of yolk at the midpoint with a tripod micrometre.
c) $\text{Yolk index} = \frac{\text{Height of yolk}}{\text{Width of yolk}}$.
d) Albumin heights were measured from at least three places each with tripod micrometre (Froning and Frank, 1956)[5].
e) Albumin width was measured as the widest horizontal circumference of the thick albumin with a Vernier calliper in centimetre.
f) $\text{Albumin index} = \frac{\text{Height of albumin}}{\text{Width of albumin}}$.
g) Shell thickness of dry egg shell was measured with a micrometre screw gauge. The average of three points (the broad, middle and narrow) were taken as shell thickness.
h) Haugh unit was determined using the following formula.

$HU = H + 7.57 - 1.7\ W^{0.37}$

Where HU = Haugh Unit
H = height of albumin (mm)

W = weight of egg (g)

Individual Haugh Unit (Haugh, 1937)[6] score was calculated using egg weight and albumin height (Doyon et al., 1986)[7]. The mean values were calculates for each trait, according the Snedecor and Cochran (1994)[8].

i) Subsequently, the yolk was segregated from albumin and measured. The weight of shell was measured after the removal of remaining albumin with water and rapid sun drying for six hours.

j) The weight of albumin was evaluated by subtracting the weight of yolk and shell from the weight of whole egg.

Chemical Analysis

Chemical analyses were carried out in two accredited laboratories namely the Feed Analytical laboratory of Central Poultry Development Organisation (CPDO) and Zoology Laboratory of Centurion University of Technology and Management located at Bhubaneswar.

In the laboratories the eggs were kept in refrigerator at 4^0C and analysed with in four days after laying. Analyses were carried out in two categories, i.e., with shell and without shell.The parameters namely energetic value, carbohydrate, cholesterol, crude protein, crude fat (lipid), moisture content, total ash, calcium and phosphorus content were determined. The cholesterol content was analysed enzymatically by using Coral Diagnostic Cholesterol Reagent as described by (Allain et al., 1974)[9]. The crude fat content was analysed by Soxhlet Extraction method as described by AOAC (1990)[10]. Similarly crude Kjeldahl method the moisture content protein was estimated by multiplying 6.25 to nitrogen content obtained by Micro- was determined by drying at 100-102^0C for 16 to 18 hours as described byAOAC (1990)[10] and ash content was analysed by incineration in muffle furnace at 550^0C.

Calcium was analysed by potassium permanganate titration method (Tee et al., 1987)[11] and phosphorus content was determined by colorimetric method using ammonium molybdate solution as described as AOAC (1990)[10]. Energetic value and carbohydrate were calculated computationally using the following formula as followed by (Matt et al., 2009)[12], i.e., Kcal/100gm of edible egg =(gm protein x 4.63) + (gm lipids x 9.02) + (gm carbohydrate x3.87)and 100% - (protein% + fat% + humidity % + ash%) respectively.

Statistical analysis

The data were analysed as per standard statistical protocol (Snedecor and Cochran, 1994)[13]. The different egg quality traits and chemical composition of eggs of both the species were studied and the mean was analysed using the t-test. Values of nutritional parameters were compared and standard error of mean were calculated using t-test and significance of test was calculated ($P < 0.01$) at 1% level.

RESULTS

External egg qualities

Generally eggs of birds have elliptical shape with small differences among species. In spite for small differences, the egg shape is considered to be an important factor in characterizing avian species. In this study, eggs of chicken showed an elliptical shape with having a rounded sharp end. The colour of chicken ranged from white to light brown. The shape of the egg is expressed in terms of shape index and the shape indices of chicken with significant statistical difference ($P < 0.01$) (Table 1). The weights of chicken egg and their components are recorded (Table 1). The Vanaraja egg weight was much higher than that of V_2 chabro egg. The proportion of yolk and albumin to the weight of whole egg are significantly higher ($P < 0.01$) in V_2 chabro (Table1). The shell of V_2 chabro egg was observed to be significantly thicker 0.047cm than the Red Cornish egg 0.040cm.

Interior egg qualities

The yolk index, albumin index and Haugh Unit of the eggs of V_2 chabro were found to be significantly higher ($P < 0.01$) (Table 1). Analysis of chemical composition of different indigenous species of chicken showed significant

differences (P < 0.01). The moisture content of Red Cornish showed highest with 77.64 while black rock have the highest protein content of 11.56 and the Dhelem red have the highest lipid content of 11.92. The energetic content value of V_2 chabro was highest than other indigenous species with 178.92 (kcal/100g) and Red Cornish has the highest carbohydrate content of 6.96.

DISCUSSION

The shape indices in the present study were higher than those reported by some authors for Vanaraja egg [14].The absolute weights of albumin ,yolk and shell weight were recorded to be significantly higher in V_2 chabro than that of other indigenous species. Since yolk index and Haugh Unit are indicators of internal egg quality and those were reported to be higher in V_2 chabro eggs, hence eggs of these species are of better quality. The higher the Haugh Unit and yolk index, the more desirable is the internal quality of the egg [15-18]. The prominent chemical compositions in the present study of chicken egg were similar to those obtained by USDA, (1983)[19] where the moisture content, crude protein crude fat and ash content were 74.57% , 12.14%, 11.5%, 0.99% respectively which is comparable with the present study.

CONCLUSION

Egg composition is not a uniform attributes and depends on many factors such as the hen breed and age. In the present study all the five indigenous species of Gallus gallusdomesticus produced eggs of acceptable external and internal quality. HoweverVanaraja have the highest egg weight, egg volume, egg width, and yolk weight. But in V_2 chabro have the lowest egg weight, egg volume , albumin length ,albumin height, yolk length, yolk height. Red Cornish have the highest moisture content, while black rock have the highest protein content and Dhelem red have the higher lipid content than other indigenous species. Energetic value content more in V_2chabro and highest carbohydrates present in Red Cornish. In developing countries, rural poultry farming are of high importance in terms of maintenance for people living. It provides them not only the food but also at considerable amount offers the opportunity of economic support. In past the rural eggs were primarily consumed by the local people, but now a day's people from other areas tends to consumed these products. It is a known fact that rural products are one of the top rank probably due to high nutritive value for almost all age groups, an important iron source for children and a low caloric and easily digestible nutrition for adults. Rural eggs were found with higher egg shell, higher egg yolk weight and higher haugh unit and can be considered as with high nutritional value as compared to commercially produced eggs[20].

ACKNOWLEDGEMENTS

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Table I. Summary of External Characters Of Indigenous Species Of Hens

Name Of The Species	Vanaraja	Red Cornish	Dhelem Red	Black Rock	V_2 Chabro
No.Of Observations	10	10	10	10	10
Egg Weight(G)	61.23±0.31**a**	56.815±0.17**a,B**	58.80±0.28**a,B,C**	52.981±0.03**a,B,C,D**	51.47±0.212**a,B,C,D**
Egg Volume(Cu Ml)	58.81±0.88**a**	54.75±0.13**a,B**	51.11±0.23**a,B,C**	49.563±0.16**a,B**	48.85±0.21**a,B,C**
Shape Index(%)	74.421±0.5**a**	65.079±1.41**ab**	75.43±0.68**b,C**	76.79±0.90**b**	80.33±0.03b**a,B,C**

*Means bearing different subscripts within rows differ significantly at P≥0.01.

Table II. Summary of Physical Characters of Indigenous Species of Hens

Name Of The Species	Vanaraja	Red Cornish	Dhelem Red	Black Rock	V_2 Chabro
Albumin Weight(G)	39.941±0.354**a**	36.83±0.585**b**	40.23±0.275**a,B,C**	30.81±0.12**c**	34.21±0.200**b,C**
Yolk Weight(G)	22.3±0.143**a**	19.98±0.024**a,B**	18.58±0.08**a,B,C**	22.14±0.037**b,C,D**	17.205±0.087**a,B,C,D**
Shell Weight(G)	7.48±0.85**a**	8.7±0.074**b**	9.24±0.15**c**	8.61±0.190**b,C**	9.23±0.109**b,D**
Thickness Of Egg Shell(CM)	0.042±0.0**a**	0.040±0.0**a,B**	0.043±0.0**c**	0.042±0.01**b,C**	0.047±0.09**c**
Albumin Index(%)	64.42±0.77**a**	87.83±1.39**a,B**	76.33±0.31**a,B,C**	78.40±0.468**a,B,D**	91.85±1.10**a,B,C,D**
Yolk Index(%)	93.27±0.79**a**	92.80±0.975**b**	92.39±0.84**c**	85.14±1.014**a,B,C, D**	95.43±0.71**d**
Haugh Unit	60.968±2.974	71.136±0.219	68.24±2.96	69.66±2.46	72.74±3.496

*Means bearing different subscripts within rows differ significantly at P≥0.01

Table III. Summary of Chemical Characters of Indigenous Species of Hens

Name Of The Species	Vanaraja	Red Cornish	Dhelem Red	Black Rock	V_2 Chabro
Moisture Content(%)	76.12±0.05	77.64±0.22	74.12±0.1	76.14±0.6	75.5±0.15
Crude Protein(%)	11.34±0.1	11.36±0.13	11.56±0.09	11.56±0.06	12.5±0.17
Crude Fat (%)	12.72±0.06	11.52±0.11	11.92±0.05	11.26±0.07	12.2±0.13
Total Ash(%)	0.96±0.04	0.36±0.05	1.1±0.1	0.9±0.04	0.48±0.11
Carbohydrate Rate(%)	0.2±0.04	0.96±0.2	0.26±0.02	0.21±0.04	0.9±0.22
Energy(Kcal/100g)	177.22±1.2	160.1±1.68	166.07±0.86	155.9±0.8	178.92±1.07

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RESEARCH ARTICLE

Induced Breeding of Gold Fish (*Carassius auratus*) using Synthetic Hormone (Ovatide) and PituitaryExtract

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ABSTRACT

The present study was intended to carry out induced breeding of gold fish (carassius auratus) in controlled environmental condition by administering ovatide, pituitary Extract and mixture of both synthetic and natural hormone at different doses. The study was conducted during the period from June to February 2020 at Department of Zoology, S.C.S (A) college, Purifor 9 months. Gold fish brooders were exposed to single dose of Ovatide @ 0.35ml/kg body weight for both female and male for induced breeding. Fecundity and hatching rate of eggs was found to be significantly higher in mixture of both natural and synthetic than the fish exposed to natural breeding and synthetic. Also, the survival rate was found to be higher in induced bred fish treated with the mixture of both natural and synthetic hormone. The hatching rate and survival success of eggs may be affected by various factors, such as temperature, water quality etc. Therefore, the optimum physio-chemical parameters of water was maintained and monitored during the entire experimental duration. The positive response of gold fish to synthetic hormone (Ovatide+pituitary) with significantly increased fecundity, fertilization and hatching rate makes it possible to conduct the breeding of this species commercially and the method can be utilized to help the farmers to increase theireconomy.

Key words: carassius auratus, Induced breeding, brooder, fecundity, hatching ovatide.

INTRODUCTION

Aquaculture is a booming sector which provides vast opportunities for entrepreneurship and livelihood generation. Ornamental fish form an important commercial component of aquaculture, providing for aesthetic requirements and upkeep of the environment. Aquarium keeping has been an age-old practice and now it is the second largest hobby in the world[1]. Introduction of civil aviation after the Second World War expanded the hobby to a global industry

[2]. In India, the concept of aquarium and aquarium fish keeping has been a practice since long, popularized mainly by the Britishers through inclusion of exotic varieties. Presently it's gaining popularity and almost every house-hold is keen to keep an aquarium in urban areas. Introduction of Chinese Vastusastra (Feng-Shui) in India adds the demand of ornamental fishes especially Gold fish which is one of the oldest and most popular hobbies in the world for ornamental fish lovers. The trade in ornamental fish has been increasing since 1980's.

Organized trade inornamental fish production depends upon assured and adequate supply of demand whichi spossibleonly by mass production through induced breeding. Induced breeding is a technique where organism is stimulated by particular hormone or other synthetic hormone or by providing condition. The stimulation promotes timely release of sperms and eggs from ripe gonads. For the first time goldfish was bred by administering human chorionic gonadotropin (HCG) in India by (Reddy et al. (1990[3].A common method used for induced breeding in fish is administration of pituitary extracts from a mammal or a fish or use of synthetic hormone [4] Goldfish is the highest traded variety not only from the standpoint of the ornamental fish trade but also as experimental test animals as it is can successfully adapt to environmental condition [5]. The present study was undertaken to develop the induced breeding technique for C.auratus using synthetic hormone, pituitary extract and mixture of both.

MATERIALS AND METHODS

Profile of the Study Area

The experiment was conducted in Zoology Laboratory of S.C.S (A) COLLEGE, Puri, under Utkal University. All preparation needed for induced breeding of goldfish were done in the laboratory. Aquarium set up, water supply facilities, working space etc. were assured before the breeding program. The experiment was done from July2019 to February2020.

Materials Requirement

1. Brooders
2. Synthetic fish breedinghormone
3. Insulin syringe
4. Woolrope
5. Aquarium
6. Small plastictop
7. Artificial greenplants
8. Potassiumparamagnet
9. Aerator
10. Air stones
11. Scoop net
12. Plankton net
13. Aquarium heater
14. Thermometer
15. PHpaper

Preparation of Rearing and Spawning Tank

For induced breeding glass aquarium was used for rearing of fish. One large size glass aquarium (4×1.5×1.5ft) were made and 1 small size plastic bath top of the laboratory were used. The aquarium was supported with filter, stone, continuous air-pump etc. The broods were conditioned in the large tank and after injecting the brood set were separated in the small bath top. After fertilizing the fertilized eggs were also kept in the smalltop.

Preparation of Spawning Top

Small top was prepared for spawning pool, so first it was washed with potassium paramagnet. The top was decoded with artificial plants and some rope, colorful stone, provide aeration by the help electricalaerator.

Experimental Design

There were two broad parts of the activities in this experiment. The first part of the activity concerned with the collection of brood fish. The second part of the experiment was performed in the zoology laboratory to carry out the induced breeding program, embryonic and larval stagedevelopment.

Brood Fish Selection, Collection and Conditioning

Mature healthy comet, fantail, gold fish brooders (90-150 g), were selected by sexual dimorphism for breeding experiments. The brood fish were selected on the basis of size and color pattern. Female is usually easier to spot, as the belly of a mature female is generally plump, whereas male remains streamlined and moretor pedoshaped. When males are ready for spawning, they develop breeding tubercles on the head and pectoral fins, principally along the bones of the fin rays. These are used during breeding, when the male nudges the female with its head and fins to induce her to spawn. 3 pairs (4 male and 2 female) brood fishes were collected from the local aquarium fish market and from the aquarium fish market of Puri and Berhampur. To increase the diversity among the parents and to select healthy brood fish, it was collected from the diversified sources. Avoiding inbreeding problem was also a major objective of selection of brood fish from diversified sources. The brood fishes were carried to the laboratory within 12 hours and kept in the aquarium (4×1.5×1.5 ft.). The brood carrying pack was submerged into the aquarium water for 10 minutes. Then the brood were unpacked and released into the well aerated aquarium (D.O: 4.5-5.5mg/L, pH: 7.2-7.4; temperature: 20-230C). The brood was kept 6-7months here before the breeding program.

Brood Stock Maintenance

Brood fish were stocked in big aquarium tanks (120ltr capacity).Before releasing into acclimatization tank, fishes were quarantined in 1ppm KMnO4 solution. Fishes were fed with supplementary feed (38% protein) at 5% of body weight twice a day, along with supplementary diet, brooders were fed earth worm on every alternative day to enhance maturity in captivity. The brood- stock was conditioned in 7-month period with intensefeeding.

Water Quality Parameter

To get optimum survival and production of aquarium fishes during the experimental period, water quality parameters were maintained at an optimum level as required for gold fish.(Table-1)

Induced Breeding

The selected broods collected from the conditioning aquarium were kept on separate aquarium. Continuous air flow was provided in the tanks by aerator. The sex ratio of the spawners was kept at 4:2 for male and female. The breeding program was conducted by a synthetic hormone (ovatide) administration. The selected brood was weighted in the electric balance and then the hormone was administered. The breeding set was released into separate top after the hormonaladministration.

Hormone Dose Optimization

For induced breeding synthetic hormone (Ovatide) was injected to the spawners was bought from the market. The supernatant solution of hormone was then taken for the injection. Both male and female was given single doses of injection. Both injected at the same time. The doses used in the two different sexes were listed inTable.

Method of Injection

Holds the fish firmly and inject the calculated amount of Ovatide solution intramuscularly inthe region of the caudal peduncle above the lateral line using an insulin hypodermic syringe having 40 units. Draw only required amount of Ovatide from the vial directly through the syringe and expel the trapped air, if any, with needle pointing upwards before giving theinjection.

Courtship and Spawning

After administration of Ovatide released into the spawning top. The courtship behavior was observed after 1-8 hours of hormone injection at the bottom of the breeding tank. Active participation was seen by both male and female. During mating splashing of water was observed frequently with dorsal fins seen above the water surface. Males release the milt by rubbing their body against the female by aligning on either side of the female. The adhesive eggs were deposited on submerged spawning top and were fertilized externally. Goldfishes are generally not good parents and they donot exhibit parental care, were separated from spawning tank soon after; hence brooders spawning.

Fertilization

Healthy goldfish eggs look like small, clear bubbles and can range in color from white to yellow-orange. They are also EXTREMELY sticky. The eggs are fertilized, look for tiny black specks in the eggs after the two or three days or so. Those are the eyes of the tiny fry developing inside. This is a3-day old (fertilized) goldfish egg**.** In 3 to 4 days, the eggs hatch (depending on the temperature).

RESULTS

The efficiency of hormone-induced was estimated based on parameters like fecundity, fertilization rate, hatching and survival of larvae. [6]

Gestation Period

After the eggs have attached, they hatched within a short time. If the water is warm, the eggs will hatch a couple days after being laid. If the water is still cold, the eggs may sit for a while, developing more slowly. Most of the eggs will hatch 2 to 7 days after laying.

Raising Goldfish Successfully Starts by Creating Ideal Conditions for Hatching

The Correct Temperature Is Important

The eggs should be kept at a temperature of between 70-75oF (21-24oC). At this temperature the eggs will hatch in 4 days.

Aeration Controls Surface Scum

The eggs should be aerated to ensure adequate oxygenated water is flowing around the eggs. The aeration also helps break up any scum that forms on the surface of the water.

Egg Development

After about 2 days should start to see eyes of the fry appearing. Two days laterthe fry starts to break out of their egg shells.

DISCUSSION

Induced breeding is one of the most viable techniques to cater to the ever-increasing demand of ornamental fish all year round. Wide use of synthetic hormones for induced breeding has yielded a reasonably good degree of success. In the experiment, C.auratus was successfully bred in captivity by the administration of ovatide. The present study indicates that using Ovatide at 0.35ml/kg of body weight of female is the ideal dose for inducing C.auratus in captivity. The present study also shows that fish treated with mixture of both synthetic and natural hormone increases fecundity, fertilization and hatching rate. In the present case better results were achieved with a single dose of injection. It was observed that the eggs of goldfish which were 0.8-1.1mm in diameter, were very much adhesive in nature and hatched in approximately 60- 65 hours at 25Oc.It also revealed that the colour of fertilized eggs was

initially transparent but slowly turned creamy as embryonic development gathered momentum. The yolk sac was fully absorbed after 60-65 hours at 24-25oCin case of C.auratus

CONCLUSION

The present study concludes that fecundity, fertilization and hatching rate can be substantially improved by captive breeding induced by hormone. The induced breeding experiment proves that combination of both ovatide and puitary extract inducement at a dose of 0.35ml/kg female is ideal to get better production than that can be obtained by natural breeding and ovatide. This investigation has standardized the ideal dose of ovatide hormone for induced breeding of C.auratus. The technology can boost production all year round without any crop gap, hence helpful for the farmers in better maintenance and in getting higher yields with the least input co

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Table 1. Water Quality parameters

Parameter	Optimum range
Temperature (co.)	20-24
pH	7.2-7.8
Dissolved oxygen(mg/l)	4.8-5.4
Free CO2 (mg/l)	Nil
Total dissolved solids (mg/l)	40-130

Table 2- Hormone dose optimization in both male and female fish

Serial Number	Male	Total Body Wt. (In Gm)	Calculated Given Doses (In Ml)	Female	Total Body Wt. (In Gm)	Calculated Given Doses (In Ml)
1	A	78	0.039	A	173GM	0.86
2	B	98	0.049	B	146GM	0.073
3	C	98	0.049			
4	D	71	0.035			

Table 3. Relationship between fecundity (average fecundity) and doses (ml/kg of body wt, N=6)

Sly no	Doses of pituitary Extract ()ml/ kg	Av.fecundity	Doses of ovatide (ml/ kg)	Av.fecundity	Doses of mixture Of ovatide and pituitary	Av.fecundity
1	0.55	00	0.55	00	0.55	00
2	0.5	30.5	0.5	29.66	0.5	35.66
3	0.45	82.33	0.45	81.33	0.45	97.33
4	0.4	365.33	0.4	360.33	0.4	403.33
5	0.35	595.66	0.35	601.33	0.35	687.66
6	0.3	547.33	0.3	545.33	0.3	597.66

Table 4. Relationship between fertilization rate (%) and doses.(N=6)

Sl no(N= 6)	Dos es (ml/k g of bod y wt)	Fertilization rate (%)	Doses (ml/k g body wt) Ovatide	Fertilization (%)	Doses (ml/kg of body wt)pituitary+ ova tide.	Fertilizati on rate%
1	0.55	00	0.55	00	0.55	00
2	0.5	38	0.5	39	0.5	45
3	0.45	70	0.45	70	0.45	80
4	0.4	78	0.4	76	0.4	84
5	0.35	94	0.35	94	0.35	97
6	0.3	65	0.3	63	0.3	75

Figure 1.Carrasiu s auratus

Figure 2.Ovatide synthetic hormone

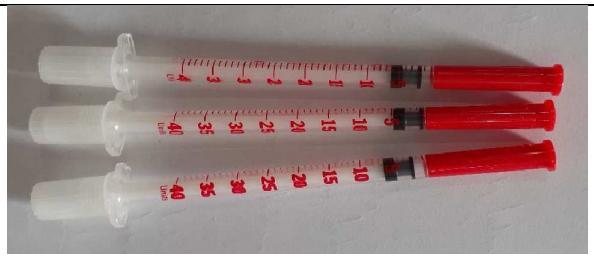
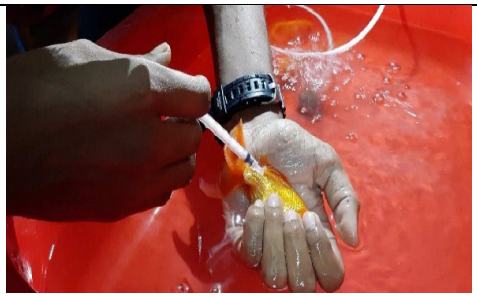
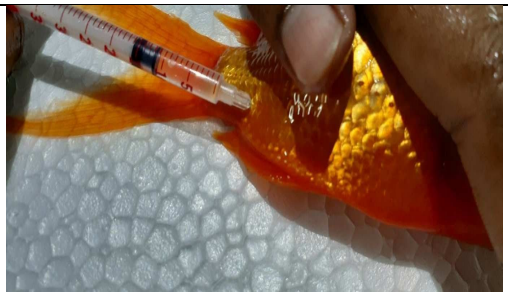


Figure 3. Insulin Syringe





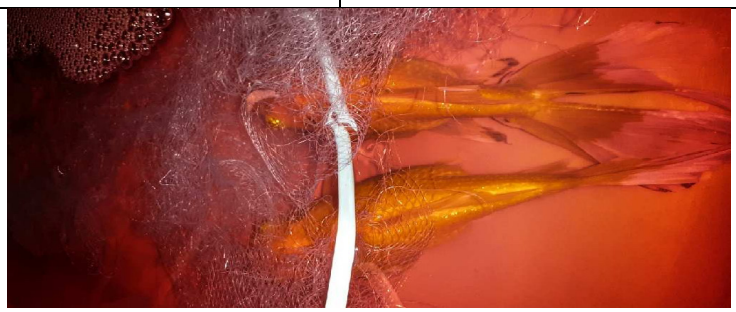


Figure 4. Injecting hormone Intramuscularly

Figure 5. 74 Hours Hatched Fry

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RESEARCH ARTICLE

Studies on Estimation of Phytochemicals from *Plumeria rubra* and *Plumeria alba*

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ABSTRACT

Pharmacognostic profile investigation of the of *Plumeria rubra* and *Plumeria alba* commonly known as Temple tree belongs to the family Apocynaceae. The investigations included the Total Alkanoid Content (TPC), Total Flavonoid Content (TFC), Total Phenolic Content (TPC). The sample were collected as leaf, bark and flower in regular month interval. Preliminary phytochemical analysis showed the presence flavonoids, alkaloids and phenolic contents. This work can be a valuable source of information of phytochemicals and can provide standards for identification of this plant material in future investigations and applications for researchers or scientists.The phytochemical content knowledge can help in field of herbal medicines in many developed and developing countries.

Keywords: *Plumeria alba, Plumeria rubra,* Phytochemicals, Plant material

INTRODUCTION

Plumeria rubra and *Plumeria alba* belong to family Apocynaceae is a sacculant, 2-8 mtr evergreen shrub having narrow elongated leaves, large and strongly perfumed white and pink flowers. Essential oil of Plumeria has antifungal efficacy and have potential for antimicrobial agents and also have pharmaceutical, anti-inflammatory, diuretic, emmengogue, febrifuge, purgative apllications and used as a tonic and expectorant[1]. Methanolic sample extract showed antimicrobial activity against *Pseudomonas aeruginosa,Bacillus anthracis*,The plant is reported to contain mixture of amyrins, amyrinacetate, scopotetin, the iriddoidsisoplumericin, plumierid ecoumerate, ß sitosterol, plumieride, and plumierid ecoumerate glucoside [2].

Nearly 80 % of the population of many developing countries are not capable to afford effective pharmaceutical drugs which based on plant, to sustain their basic health care needs which is a primary requirement [1]. In till date

medicines with herbal origin are in demand in the countries like both developed anddeveloping countries to meet basic healthcare need of people because of their vast medicinal and biological effectiveness, and also it has high safety margins than other genereic drugs and low in costs. Ayurvedic history of India has of greatknowledge on this herbal medicines which followed by tradition. The basic scientific knowledge on these traditional plants derivatives could be result clinically important. The major importance of herbal medicines seem to be their efficacy, low chances of side effects and low cost [3]. Various species of Plumeria contains different phyoconstituents. From P.acuminate leaves many phytochemicals can be isolated likelupeol acetate, lupeol carboxylic acid, stigmast-7-enol, and ursolic acid. P. rubra containing β-sitosterol-β-Dglucoside, lupeolnanoate, irroides viz. fulvoplumierin, allamcin and allamandin, as well as 2,5-dimethoxy-pbenzoquinone, (2R,3s)-3,4'dihdroxy-7,3',5'- trimethoxyflavan-5-O-β-D-glucopyranoside as Flavan3-ol Glycoside. Rubrinol; an antibacterial tritripenoid. together with teraxasteryl acetate, lupeol, stigmasterol, oleanolic acid had isolated from Bark[4].

The flower of P.rubra contains methylbenzoate, nerolidols, banzylbenzoate and methyl salicylate. The bark of P.alba containing alkaloids, flavonoids, phenolic compounds and tannins. The medicinal plant is reported to be essential by containing the iriddoidsisoplumericin, plumieride, plumieride, coumerate and plumieridecoumerate glucoside. In manystudy the antioxidant activity of methanolic extract of P. acuminate was evaluated[5].

MATERIALS AND METHODS

Collection and extraction

Leaves of *Plumeria rubra* and *Plumeria alba* were collected from GIET Campus,Gunupurand authenticated by a botanist at the Plant Anatomy Research Centre (PARC), Chennai, Tamil Nadu, India. Leaf, Bark, Flower of Plumeria of different species of different month were collected. The collection were dried in shade for 15 days and then grinded to form powder.

Phytochemicals determinationof the extract

The powder was quantitatively assessed for alkaloids, flavonoids and phenols using standard procedures as reported by Adedeji et al. (2013)[6].

Procedures

Methanol extract from the sample was prepared using Chan et al. (2006)[2] method by adding 12.5ml of methanol to 0.25gm of sample contained in a 15ml centrifuge tube and shaking, continuously at room temperature for 1 hour and 30 minutes. Methanolic extract of the sample was prepared by following the method of Chan et al. (2006) [2], by adding 12.5ml of methanol to 0.25gm of sample contained in a covered 15ml centrifuge tube and shaking , continuously for 1 hr 30 minutes at room temperature. The mixture was centrifuged at 3000-4000 rpm for 10 mins and then the supernat was collected and stored at -200c until analyse was done.

Quantification of Total Phenolic Content (TPC)

The total phenolic content was analysed by using folin-ciocalteu method [2]. 400µl of sample extract was added into the test tubes with 1.7ml of folin-ciocalteu reagent which was diluted 10times with double distilled water, and 1.4ml of Na_2Co_2 solution (7.5 w/v).The reaction was placed for 30mins at room temperature after which the absorbance was measured at 765nm against a blank prepared by distilled water. Total phenolic content was expressed as gallic acid equivalent in Mg/gm.

Quantification of total alkaloid content(TAC)

The total alkaloid contents of samples were investigated by 1, 10- phenanthroline method [7]. Sample powder (100gm) was extracted in 10 ml 80% ethanol. This was centrifuged at 5000 rpm (10 min). Supernatant were collected

to analyse the total alkaloids. The reaction mixture contained 1 mL plant extract, 1 mL of 0.025 M FeCl3 in 0.5 M HCl and 1 mL of 0.05 M of 1, 10-phenanthroline in ethanol. The blend was incubated in hot water bath (70±2 C) for 30 minutes. The absorbance of red coloured complex was measured at 510 nm. Alkaloid contents were analysed and it was calculated against standard curve of qui- nine (0.1 mg/mL, 10 mg dissolved in 10 mL ethanol and diluted to 100 mL with distilled water).

Quantification of total flavonoids content (TFC)

Aluminum chloride method [8] has been used for determining TFC. Sample (0.5 mL) of extract was dispensed into test tube, followed by 1.5 mL of methanol, 0.1 mL of aluminium chloride (10%), 0.1 mL of 1 M potassium acetate and 2.8 mL of distilled water. The reaction mixture was mixed, allowed to stand at room temperature for 30 min, before absorbance was read at 514 nm. TFC was expressed as quercetin equivalent (QE) in mg/g material.

RESULT AND DISCUSSION

Percentage extract yield

Plant tissue extraction procedures typically employ chemical ,mechanical,and/or enzymatic processes.. In this study, mechanical and chemical procedures were used sequentially with the aim of maximizing the efficiency of the extraction process. Ethanol was chosen because it has been widely recognised as suitable solvent for profiling plant tissues extracts in terms of quantity and quality.

Organoleptic characteristics of the extract

Leaves, Barks, Flowers of *Plumeria rubra* and *Plumeria alba* species produced a rough hand feel and greenish to brownish black paste with a strong alcohol smell under damp conditions while it produced a very fine elastic blackish paste with aromatic smell under dry conditions.

Phytochemicals' constituents of the extracts

In this study it was revealed that bark and flower of *Plumeria alba* contained appreciable higher phytochemicals than the *Plumeria rubra* while the leaf of *Plumeria rubra* contained higher phytochemicals than *Plumeria alba*.

Phenolic Contents

In this study it was revealed that bark and flower of *Plumeria alba* contained comparatively higher Total Phenolic content(TPC) than the *Plumeria rubra* while the leaf of *Plumeria rubra* contained less Total Phenolic content(TPC) than *Plumeria alba*. In *Plumeria rubra* the total phenolic content is higher in month of June while the content is less in month of May due to the effect of Temprature, Humidity etc.

Alkaloid Contents

In this study it was revealed that the bark and flower of *Plumeria rubra* contained comparatively higher alakaloid content Total Alkaloid Content(TAC) than *Plumeria alba* while the leaf of *Plumeria rubra* contain less Total Alkaloid Content(TAC) than *Plumeria alba*. In leaf of *Plumeria rubra* the Total Alkaloid Content(TAC) is higher in month October while the content is less in month of March due to the effect of Temprature,Humidity,Rain fall etc.

Flavonoid Contents

In this study it was revealed that the bark and leaf of *Plumeria alba* contained comparatively higher Flavonoid content Total Flavonoid Content (TFC) than *Plumeria rubra* while the leaf of *Plumeria alba* contain less Total Flavonoid Content(TFC) than *Plumeria rubra*. In leaf of *Plumeria rubra* the Total Flavonoid Content (TFC) is higher in month July while the content is less in month of March due to the effect of Temprature,Humidity, Rain fall etc.

CONCLUSION

In this study, regular harvesting of Plumeria extract was readily obtained on a monthly basis as it stooled and pollarded mother plants.. Stooling and pollarding ensured fresh and sufficient quantity that can be explored for commercial use as Plumeria protectant. The air-dried extract subjected to mechanical and chemical extraction processes sequentially yielded appreciable quantity of 5.67% ± 0.04 (n ¼ 4) ± S.D.The result (yield obtained) indicated ethanolic extraction of the Plumeria extract was able to produce enough extract for the purpose of sample treatment. Organoleptic assessment produced important characteristics such as desirable colour, odour and texture including miscibility which are of useful preservative characters.

Remarkable variations were observed between the colour, odour, and texture of the extract under the damp and dry conditions. The brownish black colour obtained suggested that Plumeria extract biomasspredominantly contained brown and black colouring pigments. The extract was found to produce burning smell under damp condition and strong burning smell (odour) under dry condition. Texture of the extract exhibited fine hand slippery feel under damp condition and formed very fine thick elastic paste under dry condition. The result suggested that the Plumeria extract contained copious amount of organic soluble oils. Chemical composition showed greater bioactive compounds in the leaf and flower compared to bark indicating the physiological defense role of stem that could have probably had greater protective impact on sample if harnessed in sufficient quantity. None readily bio-obtainability of the leaf and bark limited its use for wood treatment and antidegradation tests. Leaf extract contained 3.694 ± 0.32 mg/g total alkaloids as highest,2.61 ± 1.15 total phenol, and 0.096 ± 0.02 total flavonoids. The differences in amount of chemical compounds could be due to both intrinsic and extrinsic factors such as age, nutritional status, place of nativeness, environmental conditions, storage period etc. As expected, test block wood samples both of which are white wood contained very small or little amount of chemical compounds confirming them non-durable and suitable as reference test wood species.

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Conflict of interest

We declare that we have no conflict of interest.

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Table 1- Comparison Analysis between Bark of Plumeria SP

Bark of the species	Phytochemicals Contents		
	Phenolic	Alkaloid	Flavonoid
P.Rubra	2.035	3.116	0.16
P.Alba	2.389	3.689	0.15

Table 2- Comparison Analysis between Flower of Plumeria SP

Flower of the species	Phytochemical contents		
	Phenolic	Alkaloid	Flavonoid
P.Rubra	2.427	3.969	0.016
P.Alba	2.473	3.891	0.199

Table 3-Comparison Analysis betwwen Leaf pf Plumeria SP

Leaf of the species	Phytochemical contents		
	Phenolic	Alkaloid	Flavonoid
P.Rubra	2.777	3.189	0.089
P.Alba	1.494	3.759	0.025

Table 4 Comparision Analysis betwwen Leaf of Plumeria rubra

Leaves of *Plumeria rubra*	JAN	FEB	MAR	APRIL	MAY	JUNE	JULY	AUG	SEPT	OCT	NOV	DEC
Phenolic content	2.476	2.916	2.776	NA	1.974	3.307	3.186	NA	NA	2.777	NA	NA
Alkaloid Content	3.396	3.356	3.3125	NA	3.365	3.694	3.3678	NA	NA	3.912	NA	NA
Flavonoid content	0.016	0.096	0.078	NA	0.091	0.096	0.0996	NA	NA	0.016	NA	NA

Fig 1. Methanolic Extract of Plumeria SP

Fig 2. Preserved Extract in -4^{0}C

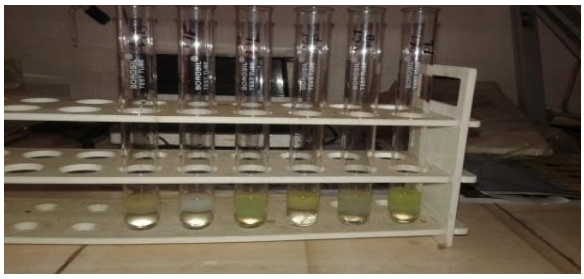


Fig 3 Phenolic extract of Plumeria SP

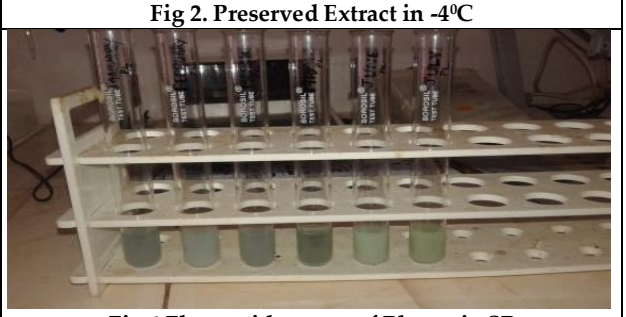


Fig 4 Flavonoid extract of Plumeria SP

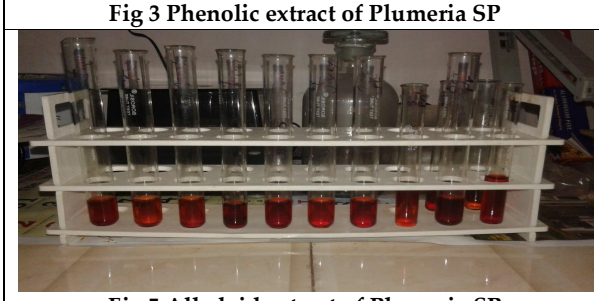
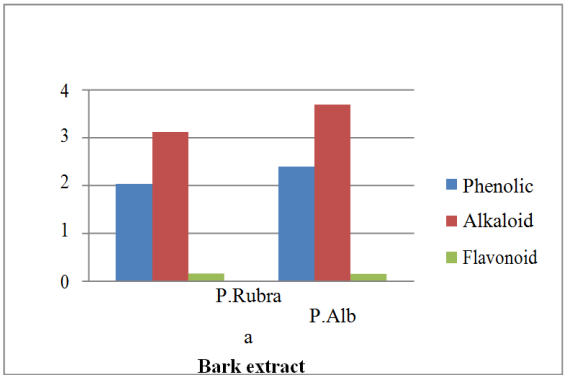
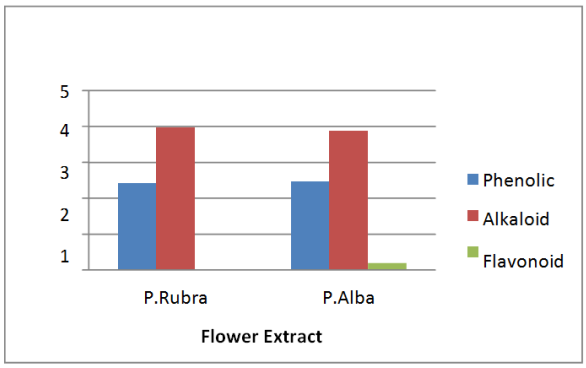


Fig 5 Alkaloid extract of Plumeria SP

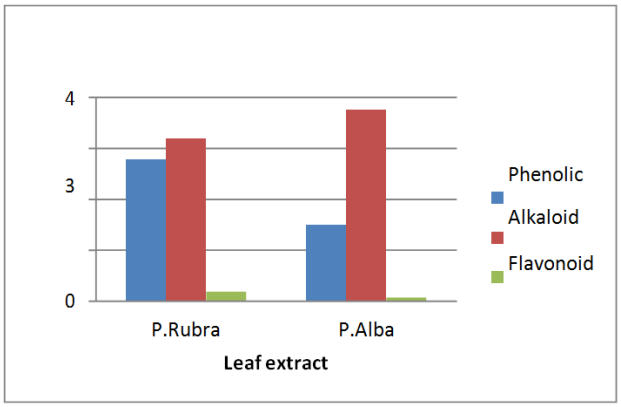
Fig 6. PAFE and PRFE



Graph 1. Bark of Plumeria SP



Graph 2.SP Flower of Plumeria



Graph 3. Leaf Plumeria SP

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RESEARCH ARTICLE

Bamboo Handicraft and Tribal Economy: A Case of Mahali Tribe of Angara Block, Jharkhand

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ABSTRACT

India has the biggest devolution of innate populace on the planet. The innate are the offspring of nature and their way of life is melded by the eco-framework. India because of its various biological systems has a wide assortment of ancestral populace. The inborn painstaking work are particular aptitudes which are given starting with one age then onto the next and these crafted works are methods for money of the craftsman. Be that as it may, without any sorted out action in this part and the items not being enough gainful, there is a potential pay of the craftsman taking up interchange economy choices (which may include movement also). In such a case this well established movement will kick the bucket its own demise. At this stage it is basic to comprehend the issues looked by this division and propose the systems for advancement of ancestral craftsmanship dependent on which certain approach level intercessions should be taken by the administration to support the conventional inborn handiworks. This undertaking discovers various issues related with Mahali experts occupied with delivering bamboo painstaking work in the towns of Jharkhand. The principle goal of the examination is to survey the bamboo make as economy alternatives for the Mahali innate network of towns, Angara, Jharkhand. Mahali has a recognized specialty legacy. Their uncommon imaginative aptitude has been smoothed out in the production of perfect family unit pieces. Not with standing, the craftsman network faces various issues and need intercession to improve their personal satisfaction. The examination features that the network

of the contemplated town experiences the gracefully of crude materials, gainful showcasing opportunity, appropriate abilities and mindfulness identified with item improvement. This venture, through essential research likewise discovers other auxiliary and utilitarian issues related with the network and recommends arrangements which can be extrapolated for various craftsman network.

Keywords: biological, network, craftsman, economy

INTRODUCTION

The craftsmen are a significant segment of our general public. By giving us perfectly made items, they upgrade our stylish life. Other than they are huge supporter of our national economy. Our handiworks have cut out a unique specialty in both created and creating nations. The term 'craftsman' is utilized to allude to those individuals who work with conventional or straightforward apparatuses to make things of fundamental need. They for the most part utilize the locally accessible assets and make important items without the guide of machine. Craftsmen generally work in conventional and disorderly area in which they are powerless against misuse and low wages. (Ansari, 2014). In India make isn't just an industry however the produce is seen as a creation representing the inward want and satisfaction of the network. Specialty Council brings up that no Indian art is ever absolutely brightening. While painstaking work, be it metal product, ceramics, mats, wood-work or weaving, satisfy a constructive need in the day by day life of individuals (Sood, 1999). High quality exercises have been remembered for family unit enterprises and labourers occupied with a portion of the administration exercises of craftsman bunch have been treated as different specialists. The fundamental measures of family unit ventures are the investment of at least one individual from family unit. This division may cover financial exercises, for example, creation, preparing, overhauling or fixing of articles or merchandise, for example, handloom, weaving, colouring, carpentry, bidi, moving earthenware producing, bike fixing, blacksmithing, fitting and so forth relying on the spot of their works the whole craftsmans works might be gathered under family and non-family sector. (Bhakare, 2016). Bamboo craftsmanship area is dominating in the Indian painstaking work and there are a huge number of individuals who rely upon bamboo for part or the entirety of their pay. The craftsman was a significant factor in the condition of Indian culture and culture. The Village people group of skilled worker have consistently been the focal point of the customary artworks of India. The station framework forced by the code of Manu protected the antiquated conventions and forestalled, or if nothing else held within proper limits, the debasing impact of outside idea. For the improvement of a less evolved state like Jharkhand, it is important to teach individuals and to prepare them in different ability and art so as to improve their everyday environments.

METHODOLOGY

The study has been carried out in the framework of villages of Angara Block, Ranchi District under Jharkhand. The Preliminary information about the block has been gathered from the Block office and secondary sources. The data for this study has been collected from Bisa, Jonha, Lupung, Gitalsud and Maheshpur villages of Angara block under Ranchi district of Jharkhand. The village was selected purposively. The independent variables which were taken for measuring the findings of the research were age, family size, family education index, family occupation & individual income.

A. Socio-economic status of the Mahali tribes

This table shows the analysis of the total population of Mohali families. In villages, 56% male and 44% female, they were depended only on Bamboo craft for their livelihood.

Age-wise analysis reveals that almost majority of the artisans in the block comes under the age group of 31-40 years (38.75%). As a matter of fact, more than half of the artisans engaged in making decorative art from bamboo were aged people in the age group of 41-60 or above i.e. 57.50%. The young age group also engaged in handicraft activities on good number i.e. 25% and 27.5%. Most of the artisans involved in bamboo handicraft activities belong to the economically weaker sections of the society. In villages, most of the bamboo handicraft artisans (100%) reported to belong to below poverty line status of the economy. The analysis of educational status of the handicraft artisans presented a very interesting picture. Most of the bamboo handicraft artisans in the village are illiterate (50%). 20% handicraft artisans reported to have received education from class 1-5, 22.5% handicraft artisans reported to have received education from class 6-8 and 7.5% handicraft artisans reported to have received education from class 9 and above.

As indicated in the table alongside, in most of the handicraft artisan households (90%) handicraft activity was reported as the main occupation. In some households, however, handicraft activity has been taken up as alternative livelihood activities to augment family income. 10% handicraft artisans reported that handicraft activity was taken up as secondary occupation for them. In some households, handicraft activity was not reported as main occupation even if the contribution of handicrafts to the annual family income was reported as higher than from other sources. This was attributed to the time the family spent on agriculture and other allied activities in the whole rather than on handicraft activities. In case of women and especially in the case of embroidery, knitting and stitching it was reported that the time left after completing household chores was used for making handicraft items as it contributed to the family income. In bamboo handicraft activity like sup, dowra, Kachi and tokari all the hanidcraft artisans reported that handicraft activities were the main occupation for them. In case of other handicraft activities most of the handicraft artisans said that handicraft activities were their main occupation.

As indicated in the table alongside, in most of the 60% handicraft artisan households were land less, 27.5% handicraft artisan households were marginal land, 8.75% handicraft artisan households were small land and 3.75% handicraft artisan households were large land. The handicraft artisans were mainly practice to agriculture cropping pattern for only house consumption purpose. In the villages of Angara block there was much difference between males and females as far as contribution to handicraft activities is concerned. There was a significant difference in contribution to handicraft activities between males and females. In villages males contribute 81.25% to all the handicraft activities whereas females contribute 18.75% to the handicraft sector. In other activities like household work, labour work, women contribute equal or more than equal to men whereas in handicraft activities like tokari, sup, and dawara making and painting, women were found to be less involved.

B. Economics of bamboo handicraft products

The table highlights the distribution of respondents on the basis of monthly income (No=80). It was observed from this table that majority of the artisans i.e. 81.25% were having average monthly income of Rs- 2000 – 4500 followed by 4600 – 7000 and 7100 - 10000 per month (15 % and 2.50%), only 1.25 percent of the artisans were having more than 10000 rupees income per month. The main reason behind it was lack of marketing opportunities. This table also shows that the standard of leaving is so poor due to low economic status of the household. This art is still continuing despite all odds faced by these tribal households. This section mainly brings out with various types of handicrafts made by these tribals and problems faced by these households. The raw materials for handicraft articles were collected from Bisa (Beti), Jonha, Lupung, Gitalsud and Maheshpur villages. The local bamboo procured from mainly four village forested areas viz. Bisa, Lupung, Gitalsud and Maheshpur but the *barlanga* bamboo could only be obtained from Jonha forest. The costs of local or *dehati* bamboos were Rs.30 per piece whereas *barlanga*/Pahari bamboo was procured from dense forest. These table reflects the marketable price or sale price of the products such as sup was Rs.40-80 per piece, Small *Khacha* was Rs.200-300 per piece, Big *Khacha* was Rs.300-500 per piece *Dowara* was Rs.200-300 per piece, *Panka* was Rs.15-20 per piece and Small *Tokri* Rs.50 per piece, Big *Tokri*was Rs.100 per piece, *Japa*was Rs.100 per piece, *Toki* was Rs.30-40 per piece, *Chala* was Rs.100 per piece, *Dela* was Rs.50-60 per piece,

*Jaru*was Rs.30 per piece, *Bawni*was Rs.20-30 per piece, *Chata* was Rs.200 per piece, *Tupa* was Rs.25 per piece and *Harka* was Rs.60-80 per piece.

The above table display the month wise production of bamboo crafts. In peak months of *Paus* to *Chaitra* (January - April) basketry products are more primed and during this period they earn the most from the basketry products but cost is not identical throughout the year, it falls down in the month of *Baisak* (May) and reaches the minimum in the months of *Ashar* (June-Jully) and *Sravana* (Jully-August) and again increase during *Kartick* (October-November) to Paus (December-January). During the month of *Ashar* (June-Jully) and *Sravana* (Jully-August) they partially remain engaged in agricultural activities, as a result of which, their productions of bamboo-work dwindle very much. During the non-agricultural season, they fully exist on basketry products as well as occasional participation in other supplementary occupation like, hunting, fishing and procurement of wild products and rarely as wage earners. *Dowara* and *Harka*was mainly used in marriage occasion and Small *Khacha*, Big *Khacha* was used for seeds storage.

CONCLUSION

Troubles in creating bamboo crafted works in the eastern territories like Jharkhand have created numerous fruitful techniques in creating and improving their bamboo painstaking work. The artworks are quality items made locally by utilizing common materials, took into account the network's needs and are progressively tough and sturdy by actualizing regular materials and propelled information on new safe materials and strong by executing normal materials and propelled information on new safe materials and strategies that will help spare the earth and help the skilled worker and network accomplish maintainable monetary turn of events. Inventive thoughts were likewise used to make new items by receiving and changing conventional kinds of artworks and transforming them into valuable family things, blessings, trinkets and toys. These new items despite everything save conventional examples, styles yet have been esteem included by finding another utilization and market for nearby social fortunes. The vast majority of the craftsmans having a place with poor foundation need back up their monetary status through giving them current method since they face the troubles in expanding the item amount in the market. The interest situated preparing would give more pay to the families. Hence there need a solid support with the state government to actualize the program for craftsman at the grassroots level and their financial status increments in the general public.

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Table 1: Total population of male and female:0

Sl. No.	Gender	Population	Percentage (%)
1	Male	223	56%
2	Female	174	44%
3	Total	397	100 %

Table 2: Age-wise distribution of handicraft artisans:

Total Artisans	21-30	31-40	41-50	51-60	> 60 years
80	12 (15%)	22 (27.5%)	31 (38.75%)	14 (17.5%)	1 (1.25%)

Table 3. Poverty status-wise distribution of handicraft artisans:

Handicraft Activity	Total Artisans	BPL
Bamboo craft	80	100%

Table 4: Education-wise distribution of handicraft artisans:

Total Artisans	Illiterate	Class 1-5	Class 6-8	Class 9 & above
80 (100%)	40 (50%)	16 (20%)	18 (22.5%)	6 (7.5%)

Table 5. Artisans involved in handicraft activity as their main or secondary occupation:

Handicraft Activity	Total artisans	Main Occupation	Secondary Occupation
Bamboo craft	80 (100%)	72 (90%)	8 (10%)

Table 6. Land holding-wise distribution of Bamboo handicraft artisans:

Total number of artisans	Land Less artisans	Marginal land artisans	Small land artisans	Large land artisans
80 (100%)	48 (60%)	22 (27.5%)	7 (8.75%)	3 (3.75%)

Table 7. Gender-wise distribution of Bamboo handicraft artisans:

Handicraft activity	Total artisans	Male	Female
Bamboo Craft	80	65 (81.25%)	15 (18.75)%

Table 8: Distribution of respondents on the basis of monthly income(N=80):

Sl. No.	Income per Month (in Rs.)	No. of respondents	Percentage
1	2000 - 4500	65	81.25
2	4600 – 7000	12	15.0
3	7100 - 10000	02	2.50
4	Above 10000	01	1.25
5	Total	80	100

Table 9: Detail about raw materials

Sl. No.	Source of raw materials (village)	Type of raw materials	Cost of raw materials
1	Bisa (Beti)	*Dehati* Bamboo (local type)	Rs 30 per piece forest collection
2	Jonha	*Dehati* (local type), *Barlanga* / *Pahari* Bamboo	Rs 30 per piece forest collection
3	Lupung	*Dehati* Bamboo (local type)	Rs 30 per piece forest collection
4	Gitalsud	*Dehati* Bamboo (local type)	Rs 30 per piece forest collection

Table 10: Bamboo by-products

Sl. No.	Type of Products	Market Price / Selling Price
1	*Sup*	Rs.40-80 per piece
2	Small *Khacha*	Rs.200-300 per piece
3	Big *Khacha*	Rs.300-500 per piece
4	*Panka*	Rs.15-20 per piece
5	Small *Tokri*	Rs.50 per piece
6	Big *Tokri*	Rs.100 per piece
7	*Dowara*	Rs.200-300 per piece
8	*Japa*	Rs.100 per piece
9	*Toki*	Rs.30-40 per piece
10	*Chala*	Rs.100 per piece
11	*Dela*	Rs.50-60 per piece
12	*Jaru*	Rs.30 per piece
13	*Bawni*	Rs.20-30 per piece
14	*Chata*	Rs.200 per piece
15	*Tupa*	Rs.25 per piece
16	*Harka*	Rs.60-80 per piece

Table11. Month-wise products of Bamboo craft:

Sl. No.	Months	Items produces
1.	Paus to Chaitra (January to April)	Small *tokri*, Big *tokri*, *Japa*, *Jaru*, *Sup*, *Chala*, *Toki*, *Harka*, *Bawni*, *Tupa*, *Dowara etc..*
2.	Baisak to Sravana (May to August)	*Panka*, Small *tokri*, Big *tokri*, *Jaru*, *Sup*
3.	Bhadra to Agrahayan (September to December)	*Sup*, Small *tokri*, Big *tokri*, Small *Khachha*, Big *Khachha*, , *Sup*, *Chala*, *Toki*, *Harka*, *Bawani*, *Dowara*

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RESEARCH ARTICLE

Skill Development and Employment Generation through Lac Cultivation in Tribal area of Ranchi District

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ABSTRACT

The study is based on the data collected from randomly selected 100 households (trained and untrained) through well-structured questionnaire and personal interview method.The study revealed that there was positive impact of training on lac growing households in terms of host utilization, livelihood conditions, and income and employment generation. The host utilization has been found to increase significantly after training of households in comparison to untrained households. A significant shift from lower production group to higher production group has been observed by trained households. Higher level of broodlac production was resulted in self-sufficiency in broodlac and more utilization of host trees for lac cultivation. The disposal pattern of crop outputs was found the same because due to lack of organized market, both the trained and untrained households sell their product in the local market. Households utilized the technologies in lac cultivation such as phunki lac removal was adopted by 100% households.Thus, the dissemination of lac cultivation technologies and strengthening of value chain and farmers' industry linkages may play a key role to harness the opportunities available for the forest and sub-forest dwellers, lac processors, manufactures, exporters and other stakeholders. Gainful

employment can be generated for migrating youths while also providing quality output to the hands of the consumer.

Keywords: Lac, Cost, Returns, Trained, Untrained, Household, Income, Employment,

INTRODUCTION

Lac is a resinous encrustation. It is produced by *phytophagous* scale insect *Kerrialacca Kerr* belongs to the family *Tachardiidae* (*Kerriidae*), superfamily *Coccoidea* of the order *Homoptera* which grow up on three commercial hosts, namely *kusum* (*Schleicheraoliosa), ber* (*Ziziphusmauritiana*) and *palas* (*Betuamonosperma*) (Govind Pal,2009; Ahmad *et al*., 2012). It is the only resinous compound of animal origin which has high economic importance due to safety for human use, it is renewable and ecosystem friendly (Ranjan *etal*., 2011). Lac is a natural resinous substance which has high economic importance in India. It is the only resin from animal origin which has diverse use. India is the country, which produce the lac more than 50% of the world's total production. Now a day an average of almost 20-22 thousand tons raw lac produced in our country. Maximum lac produced in India is from forests. (Chattopadhyay, 2011)In India, there are many lac insect species and among them *Kerrialacca (Kerr)* is used for cultivation. Two strains are, *Rangeeni* and *Kusmi* contribute 90% of the country's total lac production (Ramani, 2005). The Indian lac insect *Kerrialacca (kerr)* has two strains of lac insects are *rangeeni* and *kusmi* which have different host preference. Two crops are produced from these two strains per year. The two lac crops of "*rangeeni"* insects are *kaka* (rainy season) and *baisakhi* (summer season). *Rangeeni* strain can grow well mainly on *palas* host and some other trees also except kusum host, but *Kusmi* insects can grow well on *kusum* host and some other trees also except *palas* (Kapur, 1962; Ramani, 2005). Lac insects yields different important products like resin, wax and dye, with wide range of applications in food, adhesives, cosmetics, jewellery, paints, pharmaceuticals, perfumes, polishes varnishes and textile dyes etc. The resinous secretion (stick lac) contains about 4-5% of wax and 1% of water-soluble colouring material (lac-dye) (Dave, 1950; Sarkar, 2002; Ramani*et al*., 2007).

Lac cultivation in India

Almost 70% of the Worlds production from India and occupy the highest position in the production and export of raw lac products at the world market followed by Thailand with about 35% of the World market (Ramani *etal*, 2007).
Lac cultivation is a crucial supply of financial gain for living of the forest and sub-forest dwellers in numerous states. Besides, it's high potential for generating employment for each men and ladies in forest and sub-forest areas. In India, lac cultivation is done by village and social groups and highly practiced in the states like Jharkhand, Chhattisgarh, Orissa, West Bengal, Madhya Pradesh, Maharashtra and parts of Uttar Pradesh, Andhra Pradesh, Gujarat, and North Eastern Hill (NEH) regions (Pal, 2009). Jharkhand produce the highest lac in the country. Jharkhand contributes 58% in national lac production followed by Chhattisgarh (16.1 %), Madhya Pradesh (11.9 %), Maharashtra (5.6 %) and Odisha (3.2 %). 29% of forest area covered by the Jharkhand state (Yogi *etal*, 2014).
Ranchi, Khunti, Latehar, Lohardaga, Saraikela, Garwah West and East Singhbhum, Gumla, Simdega, Palamau, and Hazaribaghdistricts are some major lac growing districts of Jharkhand state (Chattopadhyay, 2011). In this area, the *palas*, *ber* and *kusum* are the main host plant for lac cultivation which is available. Lac production is generally found in forest and sub forest areas but now it is spreading to agriculture and waste land near the forest. Cultivation in *Semialta* has also spread quickly through seed and it has an important advantage that is its short gestation period. On an average, 39% of national lac production is contributed by this state. Ranchi is producing the highest amout (Partha and Prabhat, 2014).

Scope for the forest dwellers

Lac cultivation does not require high technology and high investment. Only part time labour is required for cultivating lac which is highly suitable for tribal people because some time they are engaged in agriculture, sometime in labour work etc. More attention by the people can lead to higher production by adopting scientific technology for cultivating lac. Lac insects are cultured on such host trees which are capable of growing in wastelands (Chattopadhyay, 2011).

Socio-economic upliftment and Employment generation through lac cultivation:

Lac cultivation is one of the most important sources of supplementary income for those who are living in forest or near the forest because the agriculture depends on rainy season only. Lac cultivation requires low investment and high profit can be achieved that is why lac cultivation is highly favourable for the tribal people. Ranchi is one of the most important lac producers in the state. Most of the STs/SCs and other economically backward communities of the district are engaged in lac cultivation.

The lac cultivation activity has high potential for generating employment for both men and women during the slack season of agriculture. Employment is generated in three stages: a) Cultivation of Lac; b) processing of Lac; and c) Trading of Lac.

Lac cultivation is done by all type of farmers i.e. marginal, small, and big also who have lac host trees *i.e..palas*, *ber* and *kusum* trees which are available in degraded land forest land, embankments unused land and plenty in the agriculture field.

OBJECTIVES OF THE STUDY

1. To study the socio economic profile of the lac growers.
2. To estimate the cost-yield analysis of lac growers.
3. To patronize and identify the constraints the problems of lac growers.

METHODOLOGY

The present study is based on the primary data collection from tribal area of Ranchi district of Jharkhand, conducted in purposively selected villages Tirlakocha, Burhakocha, Puradag, Sursu and Kuturlowa comes under Angara block of Ranchi district. It is a hilly, forested track with limited agriculture mostly paddy. Based on the information, a survey has been conducted in five villages. Finally, a total of 100 lac growers are selected and surveyed. Out of 100 lac grower, 70 trained lac growers are selected based on training exposure. For a comparative analysis of traditional and modern method of lac cultivation, 30 lac growers were selected who had not received training.

RESULT AND DISCUSSION

Socio-economic profile of the lac growers

Table 1 depicts the distribution of sampled households (trained and untrained households) across four different categories. Based on the availability of lac host tress, households were categorized in small (2-10 trees), medium (11-20 trees), large (21-100 trees) and very large (above 100 trees). It has been found that out of 100 identified households 70% household were trained and 30% were untrained. It was found that maximum household falls under medium and large category in case of both trained and untrained i.e. 36% and 35 % of the total respondent followed by 24% small and 5% very large category.

The above table shows that most of the respondents belongs to the age group of 19 to 40 years i.e. 46% of the total population followed by 41 to 60 years of age group i.e. 43 %. 9 % of the total population belongs to above 60 or aged age group. Only 2 % of the population having the age group of below 18 years.This table depicts the educational status of the respondents. Most of the respondents from both the trained (26%) and untrained (13%) categories were found illiterate i.e. 39 % of the total population followed by 26 % have received education up to class 5. 13 % of the population got their education up to class 6 -9 and 14 % have educational status up to class 9-10. Only 6 % respondent continued their education up to higher secondary level. A very interesting picture has been found from this table i.e. only 2 % of the total respondent have the education up to graduation or above and they were comes under the trained category.

Average family size of small, medium, large and very large category of both trained and untrained households is depicted in this table. In case of trained households, average family size of small category is 5.38 persons per family, followed by 5.68 persons in the medium category, 5.33 persons in the large category. Compare to the other categories, very large category have high average family size that is 6.66 persons per family.In case of untrained households, they also have high average family size that is 7 persons per family. In case of small medium and large categories they have almost same family size that are 5.83, 5.09, 5.63 persons per family.It was observed that small and medium categories have the same average family size that are 5.5 persons per family, followed by 5.42 persons in large category and 6.8 persons in the very large category. Overall average family size was found 5.54 persons per family.

Table 5 depicts the population and sex ratio of trained, untrained and pooled households. In case of trained households there are 191 males and 196 females, so the sex ratio is 97.4. In case of untrained households there are 81 males and 86 females. So the sex ratio is 94.1. Total num*ber* of male population in case of trained households is 268 and female population is 286. So the sex ratio is 93.7.The table 6 shows the experience of sampled households in lac cultivation. Overall sampled households having average experience of 9.96 years. Very large category of trained households and large category of untrained households were observed highly experienced i.e. 12.33 years and 11.02 years. Average experience of trained and untrained households was found 9.41 years and 11.23 years. In case of pooled households, it was found that the large category is highly experienced.

The above table shows average annual income of the respondents. It was witnessed from this table that majority of the farmers from Trained category i.e. 28% have the income of rupees >2 lakhs to 3.5 lakhs per annum followed by 24 % of the total respondent have the income range of rupees > 3.5 lakhs to 5 lakhs per annum. In case of untrained category 13 % of the total respondents have annual income of rupees > 3.5 lakhs to 5lakhs followed by >2 lakhs to 3.5 lakhs income range i.e. 12%. 20% of the total respondents earn up to 2 lakhs per annum from lac. Only 3% of the total population earn more than 5 lakhs per annum but they were comes under trained category witch reflects that the trained farmers were more skilled and expert of lac production and processing as compared to untrained farmers.

Proportion of available and inoculated *ber* host trees by trained households were presented in Table 8. It was evident from the table that in case of trained households, the utilization of *ber* host trees decreased in 2018-19 i.e. 36.2% in comparison to 36.5% in 2017-18. An increase was found in case of very large category of trained households from 8.8% to 9.4%. inoculation of host trees were found maximum in case of small category i.e. 91.3% in 2017-18 and 93.5 in 2018-19, followed by medium 63.1% in 2017-18 and 58.01% in 2018-19, large 33.2% in 2017-18 and 30.8% in 2018-19, very large 21.3% in 2017-18 and 23.3% in 2018-19. Table 9 depicts the available and inoculated *ber* host trees by untrained households. It was found that the utilization of *ber* host trees remains same in both the year 2017-18 and 2018-19 i.e. 92.3%. Availability of *ber* host trees found highest in case of large category but utilization was second last. It has been found that the availability of *ber* host trees in case of untrained households found very less in case of small category but the utilization of *ber* host trees was maximum that was near 90% both the year. Very less utilization of *ber* host trees were found in case of very large category that was near 21.3% in 2017-18 and 23.3% in 2018-19.

Proportion of available and inoculated *ber* host trees by pooled households were presented in **Table 10.** It was evident from the table that the utilization of *ber* host trees decreased in 2018-19 i.e. 41.4% in comparison to 43.7% in 2017-18. An increase was found in case of very large category from 21.3% to 23.3%. In case of pooled households the availability of *ber* host trees was less in case of small category but utilization was high that was 93.2% in 2017-18 and 91.3% in 2018-19.Proportion of available and inoculated *kusum* host trees by trained households were depicted in Table 11. It was evident that utilization of *kusum* host trees increased in 2018-19 (63.8%) in comparison to 2017-18 (59.0). A decrease was also found in case of large category that was from 61.8% to 57.7%. The highest increase was found in case of medium category from 49.4% to 63.5%. In both the years 2017-18 and 2018-19, maximum num*ber* of *kusum* trees was inoculated by the large category that was 60 trees in 2017-18 and 56 trees in 2018-19.

It was observed from table 12 that inoculated *kusum* lac host trees by untrained households were almost same in both the years 2017-18 and 2018-19. Small category increased the utilization of *kusum* host trees in 2018-19 (72.2%) in comparison to 2017-18. In case of medium category there was slight increase in 2018-19. Highest increase was found in case of large category from 37.5% in 2017-18 to 45% in 2018-19. But there was highest decrease in case of very large category. Table 13 depicts the *kusum* host utilization of pooled households; it was marked from the table that households increased 3.4% in 2018-19. Highest increased was found in case of medium category but they utilized only 36.0% of total lac host trees in 2017-18 and 46.6% in 2018-19. Maximum utilization of *kusum* host trees was found in case of small category. Small category utilized 69.1% in 2017-18 and 73.5% in 2018-19. Decrease in utilization of host trees was also found in case of large and very large category.

The above table shows that total inoculated brood lac by trained were decreased in 2018-19 (2557 kg) in comparison to 2017-18 (2611 kg). In case of *ber*, total inoculation was 1441 kg in 207-18 and 1392 kg in 2018-19 by all categories of households. Decrease was observed in 2018-19 in comparison to 2017-18. In case of *kusum*, total inoculation was 1170 kg in 2017-18 and 1165 kg in 2018-19 by all categories of households. Very little decrease was observed in *kusum*. In case of total (*ber+kusum*) inoculation, it was observed that small category has decreased brood lac inoculation in 2018-19 (545 kg) in comparison to 2017-18 (595 kg), followed by medium category 788 kg in 2017-18 but 787 kg in 2018-19, large category 1082 kg in 2017-18 but 1081 kg in 2018-19, very large category 146 kg in 2017-18 but 144 kg in 2018-19.
It can be noted down from the table 15 that the quantity of brood lac inoculated on *ber* trees by trained households was decreased from 17.11 kg per household to 16.05 kg per household in case of small category of households, followed by medium from 19.44 kg per households to 19.96 kg per households, large from 23.95 kg per households to 22.75 kg per households and very large from 24 kg per households to 19.33 kg per households. So only medium category has increased their brood lac inoculation of *ber* and rest categories have decreased.

Quantity of brood lac inoculated on *kusum* trees by trained households was decreased from 15.94 kg per household to 14.22 kg per household in small category of household, followed by medium from 12.2 kg per household in 2017-18 to 11.52 kg per households in 2018-19, large from 21.12 kg per households to 22.29 kg per households and very large category from 24.66 kg per households to 28.66 kg per households. Overall inoculation of brood lac in *ber* trees of all categories was 21.12 kg and 19.52 kg per household in 2017-18 2018-19. Overall inoculation of brood lac in *kusum* trees was 18.48 kg and 19.17 kg per household in 2017-18 and 2018-19. Average inoculation by trained households in 2017-18 was 39.60 kg per household in *ber* and *kusum* trees. Average inoculation by trained households in 2018-19 was 38.54 kg per households in *ber* and *kusum*. So we can conclude that trained household has decreased their brood lac inoculation.Table 16 display that total inoculated brood lac by untrained households were increased in 2018-19 (287 kg) in comparison to 2017-18 (280 kg). In case of *ber*, total inoculation was 199 kg in 207-18 and 192 kg in 2018-19 by all categories of households. In case of *kusum*, total inoculation was 81 kg in 2017-18 and 95 kg in 2018-19 by all categories of households. Very little increase was observed in *kusum*. In case of total (*ber+kusum*) inoculation, it was observed that small category has the same amount of brood lac inoculation in 2018-19 and 2017-18 that was 188 kg, followed by medium category 373 kg in 2017-18 but 354 kg in 2018-19, large category 353 kg in 2017-18 but 410 kg in 2018-19, very large category 205 kg in 2017-18 but 287 kg in 2018-19.

It can be noted down from the table 17 that the quantity of brood lac inoculated on *ber* trees by untrained households was decreased from 17.6 kg/ household to 17 kg/household in case of small category of households, followed by medium from 29.5 kg/household to 27 kg p/household, large from 22.2 kg/household to 22.7 kg/household and there was no change in case of very large category. Only large category has increased their brood lac inoculation on *ber*.Quantity of brood lac inoculated on *kusum* trees by untrained households was increased from 13.6 kg/household to 14.3 kg/household in small category of household, followed by medium from 4.3 kg/household in 2017-18 to 5 kg/household in 2018-19, large from 9.8 kg/households to 14.5 kg/household and very large category from 42.5 kg/households to 38 kg/households. Overall inoculation of brood lac in *ber* trees of all categories 32.3 kg/household and 31.6 kg/household in 2017-18 and 2018-19. Overall inoculation of brood lac in *kusum* trees was 17.5 kg/household and 17.9 kg/household in 2017-18 and 2018-19. Average inoculation by untrained household in 2017-18 was 49.8 kg/household in *ber* and *kusum* trees. Average inoculation by trained households in 2018-19 was 49.5 kg per households in *ber* and *kusum*. So we can conclude that untrained household has decreased their brood lac inoculation in 2018-19.

It was evident from the table 18 that total quantity of *phumki* lac received by trained households was increased in 2018-19 (947 kg) in comparison to 2017-18 (876 kg). The increase of phunki removal was observed in *ber* host trees that was 16.6% but there was no change in case of *kusum*. In case of small category of households there was an increase in *ber* tree (57.1%) and decrease in *kusum* (-17.3%). In medium category of households, phunki removal was found increased in case of *kusum* (8.9%) but decreased in case of *ber* (-9.0%). In case of large category of households, there was an increase in *ber* and *kusum* trees (26.4%) and (5.4%). In case of very large category of households there was no change in *ber* and a decrease was found in *kusum* (-10%). Highest increase was observed in large category of households (26.4% for *ber* and 5.4% for *kusum*). Whereas in table 19 it was perceived that total quantity of phumki lac received by untrained households was increased in 2018-19 (454 kg) in comparison to 2017-18 (441 kg). The increase of phunki removal was observed in *ber* and kussum host trees that were 1.6% and 6.1%. In case of small category of households there was an increase in *kusum* tree (63.6%) and decrease in *ber* (-36.3%). In medium category of households, phunki removal was found decreased in *ber* and *kusum* both host trees that were -7.6% and -10%. In case of large category of households, there was an increase in *ber* tree (28.2%) but there was decrease in *kusum* tree (-1.8%). In case of very large category of households, there was an increase in *ber* (27.6%) and a decrease was found in *kusum* (-8.8%). Highest increase was observed in large category of households.

It was evident from the table 20 that total produced scrapped lac by trained were increased in 2018-19 (4891 kg) in comparison to 2017-18 (4884 kg). In case of categorised groups of trained, the increase and decrease in the quantity of total produced scrapped lac was observed. Scrapped lac production on *ber* was observed decreased in all categories. In case of small and medium category, there was an increase in *kusum* tree that were 105.7% and 14.2%. In case of large and very large category, there was a decrease in *kusum* tree that were -11.9% and -6.6%. Overall it has been found that the scrapped lac production increased in 2018-19 that was 0.1%. Table 21 display that total produced scrapped lac by untrained were decreased in 2018-19 (1566 kg) in comparison to 2017-18 (1593 kg). In case of categorised groups of untrained, the increase and decrease in the total quantity of total produced scrapped lac was observed. In case of small category, there was an increase in scrapped lac production in *kusum* tree but a decrease was observed in *ber* tree. In case of medium category, there was a decrease in *kusum* tree but increase in *kusum* tree. In case of large category, there were increase and decrease in *ber* tree and *kusum* tree that were 6.4% and -8.8%. In case of very large category, there were a decrease in both *ber* and *kusum* tree that were -4.2% and -4.3%. Overall in *ber* and *kusum* there was an increase in case of large category that was 2.8%.

Quantity of produced brood lac by trained and untrained households were presented in Table 22 and 23. In case of trained farmers it was found that quantity of total produced brood lac was decreased in 2018-19 (1998 kg) in comparison to 2018-19 (2025 kg). The quantity of produced brood lac was decreased in case of small category, followed by medium and large category, it was found decreased that were -2.2% and -3.3%. In case of very large category, quantity of brood lac increased by 14.8%. Overall it was found decreased by -1.3%. Whereas in case of

untrained farmers it was observed that quantity of total produced brood lac was decreased in 2018-19 (357 kg) in comparison to 2018-19 (366 kg). Quantity of produced brood lac was decreased in case of small category by -9.6%, followed by medium, it was increased that was 10.4% and large category, it was found decreased that was -8.3%. In case of very large category, quantity of brood lac production increased by 11.5%. Overall it was found decreased by -2.4%. It was depicted in the table 24 that the total quantity of phunki lac production from *ber* trees was 498 kg by the trained households. Out of that small category produced 110 kg followed by medium category 150 kg, large category 220 kg and very large category produced only 18 kg of phunki lac. Total quantity of scrapped lac production by the trained household from *ber* trees was 3177 kg. Out of that small category produced 725 kg followed by medium category 980 kg, large category 1322 kg and very large category produced 150 kg. Total quantity of lac produced by the trained households was 3675 kg.

Total quantity of phunki lac produced from *kusum* tree by the trained household was 429 kg and total quantity of scrapped lac produced by the trained household from *kusum* trees was 1714 kg and the total amount was 1998 kg. Total quantity of brood lac production by the trained households from *ber* and *kusum* trees was 1998 kg, out of this small category produced 542 kg followed by medium 612 kg, large 720 kg and very large 124 kg only. So the total quantity of lac produced from *ber* and *kusum* by the trained households was 7816 kg and out of this small category produced 2173 kg followed by medium 2344 kg, large 2888 kg and very large category produced 411 kg. **Table 25** depicts the total quantity of lac production by trained households in kg/households. Overall phunki lac production by the trained household from *ber* trees was 7 kg/household. Scrapped lac production by the trained household from *ber* trees was 46 kg/ household and total lac production by the trained household from *ber* trees was 53 kg.

Overall phunki lac production by the trained household from *kusum* trees was 5 kg/household. Scrapped lac production by the trained household from *kusum* trees was 28 kg/household and average lac production from *kusum* was 33 kg/household by the trained household. Average brood lac production by the trained household from *ber* and *kusum* trees was 31 kg/household and total lac production by the trained households from *ber* and *kusum* including brood lac was 117 kg per household. Table 26 depicts the total quantity of lac production by untrained households. Total phunki lac production by the untrained households was 315 kg from *ber* trees followed by scrapped lac 1215 kg and the total lac production by the untrained households from *ber* trees was 1530 kg. Total quantity of phunki lac production by the untrained households from *kusum* trees was 139 kg followed by scrapped lac 351 kg and the total lac production from *kusum* trees was 490 kg. Total brood lac production by the untrained households from *ber* and *kusum* was 490 kg and grand total production by the untrained households from *ber*, *kusum* including brood lac was 2377 kg.

Table 27 depicts the total quantity of lac production by untrained households in kg/households. Average phunki lac production by the untrained household from *ber* trees was 14 kg/household. Scrapped lac production by the untrained household from *ber* trees was 49 kg/ household and average lac production by the untrained household from *ber* trees was 53 kg. Overall phunki lac production by the untrained household from *kusum* trees was 7 kg/household. Scrapped lac production by the untrained household from *kusum* trees was 19 kg/household and average lac production from *kusum* was 26 kg/household by the trained household. Average brood lac production by the untrained household from *ber* and *kusum* trees was 14 kg/household and total lac production by the untrained households from *ber* and *kusum* including brood lac was 103 kg per household.

Cost of cultivation: cost of inoculated brood lac paid by the trained households was presented in Table 28 it was revealed that total quantity of brood lac inoculated by the trained households in *ber* trees was 1186 kg and Rs.142320 paid by the trained households for 1186 kg brood lac. Highest amount paid by the large category that was Rs.61440 for *ber* trees. Total quantity of brood lac inoculated by the trained households for *kusum* trees was 878 and Rs. 105360 paid by the trained households for 878 kg of brood lac. Highest amount paid by the large category that was Rs.38400. Total quantity of brood lac inoculated by the trained households in *ber* and *kusum* trees was 2064 kg and Rs. 247680 paid by the trained category. Table 29revealed that total quantity of brood lac inoculated by the untrained

households in *ber* trees was 621 kg and Rs.74520 paid by the untrained households for 621 kg brood lac. Highest amount paid by the medium category that was Rs.29160 for *ber* trees. Total quantity of brood lac inoculated by the untrained households for *kusum* trees was 338 kg and Rs. 40560 paid by the untrained households for 338 kg of brood lac. Highest amount paid by the large category that was Rs.14400. Total quantity of brood lac inoculated by the untrained households in *ber* and *kusum* trees was 959 kg and Rs.115080 paid by the trained category. Highest amount paid by the large category for *ber* and *kusum* trees. A perusal of the Table 30 showed that highest inputs cost paid by trained households in lac cultivation activities was large (Rs. 8950) category of households followed by medium (Rs. 3005), small (Rs. 2800) and very large (Rs. 840) categories of households. Overall, it was found Rs. 15595 for the cost of other input. Apart from this, small, medium and very large categories of households were not using secateurs, nylon net and scraping knife. Table 31 showed that inputs cost paid by untrained households in lac cultivation activities was large (Rs. 660) category of households followed by small and medium (Rs. 630), and very large (Rs. 420) categories of households. Overall, it was found Rs. 2340 for the cost of other input. Apart from this, all the categorised group of households were not using secateurs, nylone net and scraping knife.

To patronize and identify the constraints the problems of lac growers

Utilization of synthetic and coupe system was not adopted by the households in the area. Households knew about these system but they did not adopted it. *Phunki* lac removal was adopted by 100% trained households as well as untrained. Out of total, 100 % of trained and 100 % of untrained households cultivated lac by pruning of lac host trees. Selection of good quantity brood lac practiced by 26% trained and 20% untrained households. Nearly 66% of trained and 37 % of untrained households adopted the technique of bundling of brood lac and tagging on plant. Only 23% of trained and 20% of untrained adopted brood lac treatments technique. 31% from trained household and 27% from untrained households use synthetic net.

The constraints faced by the trained households were depicted in Table 37. It was observed that the main problem of trained households was lac of finance for operating lac cultivation followed by climbing of lac host trees, problem of marketing facilities, shortage of brood lac and climate condition. In case of small category of households, the main problem was finance followed by climbing of lac host trees, problem of marketing facilities, shortage of brood lac and climate condition. In case of medium category of households, the main problem was finance followed by climbing of lac host trees, problem of marketing facilities, shortage of brood lac and climate condition. In case of large category of households, the main problem was found climbing of tree followed by finance, shortage of brood lac, climbing of tree and climate condition. In case of very large category of households, the main problem was finance followed by climbing of lac host trees, problem of marketing facilities, shortage of brood lac and climate condition.

The constraints faced by the untrained households were depicted in Table 38. It was observed that the main problem of untrained households was Shortage of brood lac for operating lac cultivation followed by Finance, problem of marketing facilities, climbing of tree and climate condition. In case of small category of households, the main problem was Shortage of brood lac for operating lac cultivation followed by Finance, problem of marketing facilities, climbing of tree and climate condition. In case of medium category of households, the main problem was climbing of lac host trees followed by finance problem, marketing facilities, Shortage of brood lac and climate condition. In case of large category of households, the main problem was found Shortage of brood lac for operating lac cultivation followed by marketing facilities, problem of climbing of tree, Finance and climate condition. In case of very large category of households, the main problem was Shortage of brood lac for operating lac cultivation followed by Finance, problem of marketing facilities, climbing of tree and climate condition.

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Table 1: Distribution of sampled households based on availability of total host trees (in nos.)

Categories	Trained		Untrained		Overall	
	Nos.	%	Nos.	%	Nos.	%
Small (2-10 trees)	18	18	6	6	24	24
Medium (11-20 trees)	25	25	11	11	36	36
Large (21-100 trees)	24	24	11	11	35	35
Very large (>100 trees)	3	3	2	2	5	5
Total households	70	70	30	30	100	100

(Source: field survey)

Table 2: Age group wise distribution of respondents

Category (age group in years)	Trained		Untrained		Overall	
	Nos.	%	Nos.	%	Nos.	%
Below 18	2	2	0	0	2	2
19 to 40	35	35	11	11	46	46
41 to 60	29	29	14	14	43	43
Above 60	4	4	5	5	9	9
Total	70	70	30	30	100	100

(Source: field survey)

Table 3: Educational status of the respondents

Category	Trained		Untrained		Overall	
	Nos.	%	Nos.	%	Nos.	%
Illiterate	26	26	13	13	39	39
Up to class 5	17	17	9	9	26	26
6 to 8	10	10	3	3	13	13
9 to 10	12	12	2	2	14	14
11 to 12	3	3	3	3	6	6
Graduate and above	2	2	0	0	2	2
Total	70	70	30	30	100	100

(Source: field survey)

Table -4: Family size of trained and untrained households (nos.)

Category	Trained		Untrained		Pooled	
	HH	Family size	HH	Family size	HH	Family size
Small (2-10 tree)	18	5.38	6	5.83	24	5.5
Medium (11-20 tree)	25	5.68	11	5.09	36	5.5
Large (20-100 tree)	24	5.33	11	5.63	35	5.42
Very Large (>100 tree)	3	6.66	2	7	5	6.8
Overall	70	5.52	30	5.56	100	5.54

(Source: field survey)

Table- 5: Population and sex ratio (family members) of trained and untrained households

Category	HH	Male	Female	Total	Sex Ratio
Trained	70	191	196	387	97.4
Untrained	30	81	86	167	94.1
Overall	**100**	**268**	**286**	**554**	**93.7**

(Source: field survey)

Table-6: Average experience in lac cultivation of pooled households (in years)

Category	Trained		Untrained		Pooled	
	HH	Avg. Experience (years)	HH	Avg. Experience (years)	HH	Avg. Experience (years)
Small (2-10 tree)	18	8.05	6	10.33	24	8.62
Medium (11-20 tree)	25	9.4	11	9.63	36	9.47
Large (20-100 tree)	24	10.08	11	13.09	35	11.02
Very Large (>100 tree)	3	12.33	2	12.5	5	12.4
Overall	70	9.41	30	11.23	100	9.96

(Source: field survey)

Table-7: Average annual income of respondents (in Rupees)

Annual Income Range (in rupees)	No. of Household					
	Trained	%	Untrained	%	Total	%
Below 2 Lakhs	15	15	5	5	20	20
>2 lakhs to 3.5 lakhs	28	28	12	12	40	40
> 3.5 lakhs to 5lakhs	24	24	13	13	37	37
Above 5 lakhs	3	3	0	0	3	3
Total	**70**	**70**	**30**	**30**	**100**	**100**

(Source: field survey)

Table-8: Proportion of available and inoculated lac host trees of trained households (in *ber*)

Category	HH	Available host trees (in nos.)	Inoculated host trees (in nos.)		Inoculated host trees (in %)	
			2017-18	2018-19	2017-18	2018-19
Small (2-10 tree)	18	78	73	71	93.5	91.02
Medium (11-20 tree)	25	206	112	102	54.3	59.5
Large (20-100 tree)	24	474	156	144	32.9	30.3
Very Large (>100 tree)	3	159	14	15	8.8	9.4
Overall	70	917	355	332	36.5	36.2

Table-9: Proportion of available and inoculated lac host trees of untrained households (in *ber*)

Category	HH	Available host trees (in nos.)	Inoculated host trees (in nos.)		Inoculated host trees (in %)	
			2017-18	2018-19	2017-18	2018-19
Small (2-10 tree)	6	26	24	24	92.3	92.3
Medium (11-20 tree)	11	90	75	70	83.3	78.8
Large (20-100 tree)	11	142	49	46	34.5	32.3
Very Large (>100 tree)	2	42	29	32	69.04	76.1
Overall	30	300	177	172	59	57.3

Table-10: Proportion of available and inoculated lac host trees of pooled households (in *ber*)

Category	HH	Available host trees (in nos.)	Inoculated host trees (in nos.)		Inoculated host trees (in %)	
			2017-18	2018-19	2017-18	2018-19
Small (2-10 tree)	24	104	97	95	93.2	91.3
Medium (11-20 tree)	36	296	187	172	63.1	58.01
Large (20-100 tree)	35	616	205	190	33.2	30.8
Very Large (>100 tree)	5	201	43	47	21.3	23.3
Overall	100	1217	532	504	43.7	41.4

(Source: field survey)

Table-11: Proportion of available and inoculated lac host trees of trained (in *Kusum*)

Category	HH	Available host trees (in nos.)	Inoculated host trees (in nos.)		Inoculated host trees (in %)	
			2017-18	2018-19	2017-18	2018-19
Small (2-10 tree)	18	50	35	37	70	74
Medium (11-20 tree)	25	85	42	54	49.4	63.5
Large (20-100 tree)	24	97	60	56	61.8	57.7
Very Large (>100 tree)	3	17	10	12	58.8	70.5
Overall	70	249	147	159	59.0	63.8

Table-12: Proportion of available and inoculated lac host trees of untrained (*Kusum*)

Category	HH	Available host trees (in nos.)	Inoculated host trees (in nos.)		Inoculated host trees (in %)	
			2017-18	2018-19	2017-18	2018-19
Small (2-10 tree)	6	18	12	13	66.6	72.2
Medium (11-20 tree)	11	48	6	8	12.5	16.6
Large (20-100 tree)	11	40	15	18	37.5	45
Very Large (>100 tree)	2	23	16	11	69.5	47.8
Overall	30	129	49	50	37.9	38.7

Table-13: Proportion of available and inoculated lac host trees of pooled households in (*kusum*)

Category	HH	Available host trees (in nos.)	Inoculated host trees (in nos.)		Inoculated host trees (in %)	
			2017-18	2018-19	2017-18	2018-19
Small (2-10 tree)	24	68	47	50	69.1	73.5
Medium (11-20 tree)	36	133	48	62	36.0	46.6
Large (20-100 tree)	35	137	75	74	54.7	54.0
Very Large (>100 tree)	5	40	26	23	65	57.5
Overall	100	378	196	209	51.8	55.2

(Source: field survey)

Table- 14: Quantity of inoculated brood lac by trained on *Ber* and *Kusum* (in Kg)

Category	HH	2017-18			2018-19		
		Ber	*Kusum*	Total	*Ber*	*Kusum*	Total
Small (2-10 tree)	18	308	287	**595**	289	256	**545**
Medium (11-20 tree)	25	486	302	**788**	499	288	**787**
Large (20-100 tree)	24	575	507	**1082**	546	535	**1081**
Very Large (>100)	3	72	74	**146**	58	86	**144**
Overall	**70**	**1441**	**1170**	**2611**	**1392**	**1165**	**2557**

(Source: field survey)

Table- 15: Quantity of inoculated brood lac by trained on *Ber* and *Kusum* (in Kg/hh)

Category	HH	2017-18			2018-19		
		Ber	*Kusum*	Total	*Ber*	*Kusum*	Total
Small (2-10 tree)	18	17.11	15.94	33.05	16.05	14.22	30.27
Medium (11-20 tree)	25	19.44	12.2	31.64	19.96	11.52	31.48
Large (20-100 tree)	24	23.95	21.12	45.07	22.75	22.29	45.04
Very Large (>100 tree)	3	24	24.66	48.66	19.33	28.66	47.39
Overall	70	21.12	18.48	39.60	19.52	19.17	38.54

(Source: field survey)

Table- 16: Total amount of inoculated brood lac by untrained on *Ber* and *Kusum*(in Kg)

Category	HH	2017-18			2018-19		
		Ber	*Kusum*	Total	*Ber*	*Kusum*	Total
Small (2-10 tree)	6	106	82	188	102	86	188
Medium (11-20 tree)	11	325	48	373	298	56	354
Large (20-100 tree)	11	245	108	353	250	160	410
Very Large (>100 tree)	2	120	85	205	120	76	196
Overall	30	199	81	280	192	95	287

(Source: field survey)

Table- 17: Quantity of inoculated brood lac by untrained on *Ber* and *Kusum* (in Kg/hh)

Category	HH	2017-18			2018-19		
		Ber	*Kusum*	Total	*Ber*	*Kusum*	Total
Small (2-10 tree)	6	17.6	13.6	31.2	17	14.3	31.3
Medium (11-20 tree)	11	29.5	4.3	33.8	27	5	32
Large (20-100 tree)	11	22.2	9.8	32	22.7	14.5	37.5
Very Large (>100 tree)	2	60	42.5	102.5	60	38	98
Overall	30	32.3	17.5	49.8	31.6	17.9	49.5

(Source: field survey)

Tabl-18: Total quantity of *phunki* lac production by trained (in kg) and changes in 2018-19 over 2017-18

Category	HH	2017-18			2018-19			Changes in 2018-19 over 2017-18 (in %)		
		Ber	*Kusum*	Total	*Ber*	*Kusum*	Total	*Ber*	*Kusum*	Total
Small	18	70	104	174	110	86	196	57.1	-17.3	12.6
Medium	25	165	112	277	150	122	272	-9.0	8.9	-1.8
Large	24	174	203	377	220	214	434	26.4	5.4	15.1
Very Large	3	18	30	48	18	27	45	0	-10	-6.2
Overall	70	427	449	876	498	449	947	16.6	0	8.1

Tabl-19: Total quantity of *phunki* lac production by untrained (in kg) and changes in 2018-19 over 2017-18

Category	HH	2017-18			2018-19			Changes in 2018-19 over 2017-18 (in %)		
		Ber	*Kusum*	Total	*Ber*	*Kusum*	Total	*Ber*	*Kusum*	Total
Small)	6	55	22	77	35	36	71	-36.3	63.6	-7.7
Medium	11	130	20	150	120	18	138	-7.6	-10	-8
Large	11	78	55	133	100	54	154	28.2	-1.8	15.7
Very Large	2	47	34	81	60	31	91	27.6	-8.8	12.3
Overall	30	310	131	441	315	139	454	1.6	6.1	2.9

(Source: field survey)

Table-20: Total quantity of scraped lac production by trained (in kg) and changes in 2018-19 over 2017-18

Category	HH	2017-18			2018-19			Changes in 2018-19 over 2017-18 (in %)		
		Ber	*Kusum*	Total	*Ber*	*Kusum*	Total	*Ber*	*Kusum*	Total
Small	18	750	345	1095	725	710	1435	-3.3	105.7	31.0
Medium	25	1200	420	1620	980	480	1460	-18.3	14.2	-9.8
Large	24	1425	468	1893	1322	412	1734	-7.2	-11.9	-8.3
Very Large	3	156	120	276	150	112	262	-3.8	-6.6	-5.0
Overall	70	3531	1353	4884	3177	1714	4891	-10	26.6	0.1

Table-21: Total quantity of scraped lac production by untrained (in kg) and changes in 2018-19 over 2017-18

Category	HH	2017-18			2018-19			Changes in 2018-19 over 2017-18 (in %)		
		Ber	*Kusum*	Total	*Ber*	*Kusum*	Total	*Ber*	*Kusum*	Total
Small	6	196	90	286	179	108	287	-8.6	20	0.3
Medium	11	540	60	600	510	62	572	-5.5	3.3	-4.6
Large	11	325	102	427	346	93	439	6.4	-8.8	2.8
Very Large	2	188	92	280	180	88	268	-4.2	-4.3	-4.2
Overall	30	1249	344	1593	1215	351	1566	-2.7	2.0	-1.6

(Source: field survey)

Table-22: Total quantity of brood lac production by trained (in kg) and changes in 2018-19 over 2017-18

Category	HH	2017-18	2018-19	Changes in 2018-19 over 2017-18 (in %)
Small (2-10 tree)	18	546	542	-0.7
Medium (11-20 tree)	25	626	612	-2.2
Large (20-100 tree)	24	745	720	-3.3
Very Large (>100 tree)	3	108	124	14.8
Overall	70	2025	1998	-1.3

Table-23: Total quantity of brood lac production by untrained and changes in 2018-19 over 2017-18

Category	HH	2017-18	2018-19	Changes in 2018-19 over 2017-18 (in %)
Small (2-10 tree)	6	124	112	-9.6
Medium (11-20 tree)	11	96	106	10.4
Large (20-100 tree)	11	120	110	-8.3
Very Large (>100 tree)	2	26	29	11.5
Overall	30	366	357	-2.4

(Source: field survey)

Table- 24: Total quantity of lac production by trained households (in kg) (2018-19)

Category	HH	*Ber*			*Kusum*			Brood	Grand total
		Phunki	scraped	Total	Phunki	Scraped	Total		
Small	18	110	725	**835**	86	710	**796**	**542**	**2173**
Medium	25	150	980	**1130**	122	480	**602**	**612**	**2344**
Large	24	220	1322	**1542**	214	412	**626**	**720**	**2888**
Very Large	3	18	150	**168**	7	112	**119**	**124**	**411**
Overall	70	**498**	**3177**	**3675**	**429**	**1714**	**2143**	**1998**	**7816**

(Source: field survey)

Table- 25: Total quantity of lac production by trained households (in kg/hh)

Category	HH	*Ber*			*Kusum*			Brood	Grand total
		Phunki	scraped	Total	Phunki	Scraped	Total		
Small	18	6	40	46	5	39	**44**	**30**	**120**
Medium	25	6	39	45	5	19	**24**	**24**	**93**
Large	24	9	55	64	9	17	**26**	**30**	**120**
Very Large	3	6	50	56	2	37	**39**	**41**	**136**
Overall	70	**7**	**46**	**53**	5	28	**33**	**31**	**117**

(Source: field survey)

Table- 26: Total quantity of lac production by untrained households (in kg) (2018-19)

Category	HH	*Ber*			*Kusum*			Brood	Grand total
		Phunki	Scraped	Total	Phunki	Scraped	Total		
Small	6	35	179	**214**	36	108	**144**	**112**	**470**
Medium	11	120	510	**630**	18	62	**80**	**106**	**816**
Large	11	100	346	**446**	54	93	**147**	**110**	**703**
Very Large	2	60	180	**240**	31	88	**119**	**29**	**388**
Overall	30	**315**	**1215**	**1530**	**139**	**351**	**490**	**357**	**2377**

(Source: field survey)

Table- 27: Total quantity of lac production by untrained households (in kg/hh)

Category	HH	*Ber*			*Kusum*			Brood	Grand total
		Phunki	scraped	Total	Phunki	Scraped	Total		
Small	6	6	30	**36**	6	18	**24**	**19**	**79**
Medium	11	11	46	**57**	2	6	**8**	**10**	**75**
Large	11	9	31	**40**	5	8	**13**	**10**	**63**
Very Large	2	30	90	**120**	16	44	**60**	**15**	**195**
Overall	30	**14**	**49**	**63**	7	19	**26**	**14**	**103**

(Source: field survey)

Table- 28: Cost of broodlac in case of trained (in Rs.)

Category	HH	*Ber*		*Kusum*		Total	
		Qty.	Value	Qty.	Value	Qty.	Value
Small (2-10 tree)	18	248	29760	180	21600	428	51360
Medium (11-20 tree)	25	366	43920	300	36000	666	79920
Large (20-100 tree)	24	512	61440	320	38400	832	99840
Very Large (>100 tree)	3	60	7200	78	9360	138	16560
Overall	70	1186	142320	878	105360	2064	247680

Table- 29: Cost of broodlac in case of untrained (in Rs.)

Category	HH	*Ber*		*Kusum*		Total	
		Qty.	Value	Qty.	Value	Qty.	Value
Small (2-10 tree)	6	92	11040	84	10080	176	21120
Medium (11-20 tree)	11	243	29160	56	6720	299	35880
Large (20-100 tree)	11	184	22080	120	14400	304	36480
Very Large (>100 tree)	2	102	12240	78	9360	180	21600
Overall	30	621	74520	338	40560	959	115080

(Source: field survey)

Table-30: Cost incurred on other inputs owned/purchased by trained households (in Rs.)

Category	HH	Secateurs	*Dauli*	*Nylone* net	Insecticides / Fungicide	Scrapping Knife	Total cost
Small (2-10 tree)	18	0	2800	0	0	0	2800
Medium (11-20 tree)	25	0	2520	0	485	0	3005
Large (20-100 tree)	24	1800	2450	1700	2040	960	8950
Very Large (>100)	3	0	840	0	0	0	840
Overall	70	1800	8610	1700	2525	960	15595

Table-31: Cost incurred on other inputs owned/purchased by untrained households (in R)

Category	HH	Secateurs	*Dauli*	*Nylone* net	Insecticides / Fungicide	Scrapping Knife	Total cost
Small (2-10 tree)	6	0	630	0	0	0	630
Medium (11-20 tree)	11	0	420	0	210	0	630
Large (20-100 tree)	11	0	420	0	240	0	660
Very Large (>100)	2	0	420	0	0	0	420
Overall	30	0	1890	0	450	0	2340

(Source: field survey)

Table- 36: Technology adoption of the lac growers.

Sl.	Technologies	Trained	%	Untrained	%
1	**Pruning of lac host**	70	100	30	100
2	**Selection of good quality brood lac**	18	26	6	20
3	**Bundling of brood lac**	46	66	11	37
4	**Brood lac Treatment with insecticide**	16	23	6	20
5	***Phunki* removal**	70	100	30	100
7	**Use of synthetic net**	22	31	8	27

(Source: field survey)

Table 37: Constraint faced by trained lac growers (Ranks given by the households)

Category	Climbing of tree	Marketing	Shortage of brood lac	Finance	Climate
Small (2-10 tree)	2	3	4	1	5
Medium (11-20 tree)	2	3	4	1	5
Large (20-100 tree)	1	3	5	2	4
Very Large (>100 tree)	4	2	3	1	5
Overall	2	3	4	1	5

Table 38: Constraint faced by untrained lac growers (Ranks given by the households)

Category	Climbing of tree	Marketing	Shortage of brood lac	Finance	Climate
Small (2-10 tree)	4	3	1	2	5
Medium (11-20 tree)	1	3	4	2	5
Large (20-100)	3	2	1	4	5
Very Large (>100)	4	3	1	2	5
Overall	4	3	1	2	5

(Source: field survey)

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RESEARCH ARTICLE

Screening of Bio-formulations for their Bio-Efficacy against *Trichoderma*: In Relation to Edible Mushroom

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ABSTRACT

The present investigation has been conducted on one of the major contaminants and a myco-parasitc fungus *Trichoderma* infecting various cultivated mushrooms in and around Ranchi (Jharkhand). The objective of the study was to identify some potent herbal formulations, particularly Neem-based bio-agents, by *in vitro* testing of formulations like Indo-Neem, Maha Neem, Neem Herbal, Herbal Suddhi, Nimyle, and Well Guard for their bio-efficacy against the pathogen *Trichoderma viride*. The bio-efficacy of the formulations was tested by poisoned food technique for their ability to restrict the mycelial growth and sporulation of *T. viride* on PDA plates. Replicated experiments indicated that only Well Guard was able to effectively retard both growth and sporulation of *T. viride* at 10^{-3} &10^{-4}acquous dilutions of the formulation, while Nimyle and Maha Neem were very feebly effective to restrict the pathogen at such lower dilutions. Rest of the bio-agents like Indo-Neem, Neem Herbal, and Herbal Suddhi, were ineffective against *T. viride* at dilutions tested during the experiment. Therefore, only Well Guard and Nimyle were selected as potent bio-agents against the myco-parasite *T. viride* and were further tested against two cultivated mushrooms, *viz. Pleurotusflorida,* and *Hypsizygousulmarius* at 10^{-3} &10^{-4} dilutions so as to identify the safe dilution of the potent formulation for their use in crops of mushrooms, so that the bio-agents may be used to restrict *Trichoderma viride* without any harmful effect on the growth and production of the mushroom species. Replicated *in vitro* studies on the two mushrooms by the same poisoned food technique indicated that Well Guard at 10^{-4}dilution might be safely used to manage the

Green mould fungus *T.viride* without any adverse effect on both the mushrooms, if further *in vivo* studies on their spawn preparation and crop-production are carried out. Significantly, in the present study Well Guard, which is being currently promoted as a Growth-promoting formulation containing a mixture of amino-acids and short chain polypeptides has now been identified as a potent bio-control agent for controlling a pathogenic fungus like *Trichoderma viride* causing havoc in button mushroom industry the world-over. Nevertheless, other bio-formulations tested during the study require to be further evaluated for their bio-efficacy against *T.viride* at concentrations higher than those tried during the present investigation.

Keywords : *Trichoderma*, Bio-agents and Oyster mushroom.

INTRODUCTION

In India, mushroom cultivation started only during the last century, as the Paddy straw mushroom *Volvariella volvacea* was first cultivated on paddy straw in 1940s at Coimbatore (Ahlawat*et al*, 2005) later in 1962, *Pleurotus flabellatus (Dhingri or oyster)* was successfully cultivated on paddy-straw in Mysore (Srivastava and Bano,1962). Mushrooms are grown on organic residues, from which the mushroom mycelium draws nourishment through enzymatic degradation. In this process, they face competition as well as pathogenic attacks by various fungi, bacteria, insects etc, which hamper their growth and fruiting. Studies have shown that such problems might occur at various stages. These might occur in cultures, in spawn, on mushroom beds or even on mushroom sporopheres and cause damage and loss, and their good accounts are available in the litsature (Verma 2011).Cultivation of mushroom, however, faces several problems like diseases caused by viruses, bacteria, and fungi, and infestation by insects, and mites. Of these *Trichoderma spp*. cause major problem for mushroom farming. This problem is not restricted to India alone, but spread all over the world. Some *Trichoderma* strains have developed the capability to resist some chemical fungicides, and hence several countries have banned the use of some systemic chemical fungicides in mushroom cultivation. Therefore, people are now looking for alternatives like bio-fungicides or herbal formulations, etc. for combating this wide-spread disease of mushrooms.

Neem based bio-pesticide have shown great potentials in the management of insect-pests, and some such products have also shown efficacy against microbial contaminants. It was therefore, proposed to screen different Neem-based and other commercial herbal formulations available in the market for their efficacy against *Trichoderma*, a common pathogen of mushroom cultures, spawn, beds and even the sporocarps causing huge losses to mushroom producers at every step.

METHODOLOGY

1. **Selection of Bio-Formulations :-** For this experiment I select some potent neem based or bio-agents which are available in Ranchi market i.e. Maha Neem, Indo-Neem, Well Guard, Nymile, HarbalSuddhi and Neem Harbal.
2. **Growth-Dynamics studies on *pleurotus florida, hypsizygus ulmarius* & *trichoderma viride* as influenced by respective bio-formulations:** With a view to study the growth dynamics of *Trichoderma viride* as influenced by selected six Bio-formulations, replicated experiments were laid to grow the fungus in PDA plates impregnated with different dilutions of the selected bio-agents by poisoned food technique. An untreated control without any bio-formulation was also plated. Later, only potent bio-formulation was used to test its effect on the mycelial growth of the two mushroom fungi by the same technique and procedure.
3. **Poisioned Food Technique :**In this technique, the selected bio-agents were mixed in the culture medium at different dilutions, when the sterilized agar-medium was still in molten state but cooled to around 47-50 C, so that there was no adverse effect on the efficacy of the bio-agents. The test-fungi were later inoculated in the centre of the

plates, when the medium got cooled and solidified. An untreated control was also laid by the same procedure except that no bio-agent was added in those plates.

A. TO PREPARE SERIAL DILUTIONS OF DIFFERENT BIO-AGENTS

To prepare the serial dilutions (10^{-3}, 10^{-4}, and 10^{-5}) of the Bio-formulations, 9 ml of distilled water was taken in several test-tubes, and they were sterilized at 15 lb p.s.i. pressure and were left to cool down to room temperature. Thereafter, 1 ml of the bio-product was added into the 1st .test- tube containing 9ml of sterilized distilled water with the help of a sterilized pipette and was well shaken to get 10^{-1} dilution of the Bio-formulations. Thereafter, 1 ml of 10^{-1} dilution was transferred to the 2nd test-tube containing 9ml of sterilized distilled water and shaken properly to prepare the 10^{-2} dilution of the bio-agents Likewise 10^{-3}, 10^{-4} and 10^{-5} dilutions ofdifferent bio-agents were prepared for their use in the growth dynamic studies on different test-fungi.

B. INOCULATION OF TEST-FUNGI ON POISONED MEDIUM

To inoculate the test-fungi on poisoned PDA medium, sterilized 100 mm dia. Petri-plates were taken and 1 ml of serial dilutions of different bio-agents were taken in the centre of the plates and the molten PDA medium (cooled to about 47 C)was slowly poured into the plates with sterile precautions. The plates were then gently rotated and left for 10-15 minutes to solidify. Small bit of pure culture mycelium of thetest-fungus was inoculated in the centre of each plate and incubated at 28± 1 C in BOD incubator. For each dilution of every bio-agent, 5 replicates were prepared, along with 5 replicates of control plates without any treatment. These culture plates were observed every day to record the radial growth, and days for filling the plate. For *Trichoderma viride*extent of sporulation was also recorded as radius in cm of sporulating zones in each plate.

C. STUDY ON THE EFFECT OF BIO-AGENTS ON GROWTH DYNAMICS OF TEST-FUNGI.

The treated and control plates were incubated in BOD-Incubator placed randomly in CRD at 28± 1 C and were observed every day to record the radial mycelial growth in cm till the plates were fully covered. For *Trichoderma viride,* the sporulating-zones were also measured daily as radius in cm. The data were tabulated and put to statistical analysis under CRD for testing their significance.

RESULT AND DISCUSSION

Two out of six bio-formulations tested exhibited inhibitory effect on mycelial growth and only one viz. Will Guard inhibited both growth and sporulation of Trichoderma viride (Safer doses of Well Guard (10^{-4} and 10^{-5} dilution)). Whereas Nimyle bio formulation are inhibiting the growth of mushroom mycelial and the dilution 10^{-4} and 10^{-5} dose not any inhibiting effect on mushroom mycelial growth. A perusal of data recorded in Table 1.1 and 1.2 as radial mycelial growth and sporulation growth of the fungus and the growth-pattern indicated that all Well Guard dilutions used in the experiment containing 1.5, 0.15 and 0.015 ppm Azadirachtin were highly effective to retard the mycelial growth of *T. viride* up to 3rd days of incubation, while at 1.5 ppm concentration, it retarded the growth till 5th day. Thus, that product was found to be most potent formulation to check the growth of *T. viride* during its vegetative phase. A perusal of data recorded in Table 1.1 and 1.2 as radial mycelial and sporulation growth of the fungus *T. viride* and the growth pattern exhibited that the Nimyle dilutions 10^{-3}, 10^{-4}, and 10^{-5} had only a little effect on the mycelial growth of *T.viride,* since the mycelial growth attained in treated as well as untreated control plates differed significantly only on 2nd day at 1.5 ppm and 0.015 ppm concentrations. Such little effect of Nimyle against *T. viride* recorded during the present experiment might be due to lower content of Azadirachtin in the original formulation, although the actual concentration of Azadirachtin in the formulation is not indicated.

A perusal of data in Table 1.3 recorded as radial mycelial growth of *P. florida,H. ulmarius* and *C. indica* indicated that the dilutions (10^{-3}, 10^{-4} and 10^{-5}) of Well Guard used in the experiment had significant effect on mycelial-growth of the mushroom *P. florida*and *H. ulmarius* as there was no significant difference between growth in treated and

untreated plates of *C. indica* mushroom mycelium. Mahto and Verma (2008) also recorded no adverse effect of Venguard on mycelial growth of *Pleurotusflabellatus* both *in vitro* and *in vivo* studies. T= Treatment, T.V = *Trichoderma viride*, P.F = *Pleurotusflorida*, H.U= *Hypsizygousulmarius*, C.I = *Calocybeindica*.

CONCLUSION

The present investigation has been conducted on one of the major contaminants and a myco-parasitc fungus *Trichoderma* infecting various cultivated mushrooms in and around Ranchi (Jharkhand). Therefore, only Well Guard and Nimyle were selected out of sex bio agents as potent bio-agents against the myco-parasite *T. viride* and were further tested against three cultivated mushrooms, *viz. Pleurotusflorida*,*Hypsizygusulmarius*and *C. indica* at 10^{-3} &10^{-4} dilutions so as to identify the safe dilution of the potent formulation for their use in crops of mushrooms, so that the bio-agents may be used to restrict *Trichoderma viride* without any harmful effect on the growth and production of the mushroom species. Replicated *in vitro* studies on the three mushrooms by the same poisoned food technique indicated that Well Guard at 10^{-4}dilution might be safely used to manage the Green mould fungus *T.viride* without any adverse effect on both the mushrooms,

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Table 1. Mycelial growth of *Trichoderma viride* as influenced by Nimyle and Well Guard dilution.(Treatment)

			Well Guard			Nimyle		
			Days of Incubation			Days of Incubation		
			1 Day	2 Day	3 Day	1 Day	2 Day	3 Day
(Treatment)	Radial growth (Mean in mm)	**10^{-3}**	4.00 *	17.00 *	27.80 *	11.6	33.80 *	45.60
		10^{-4}	7.20 *	33.00 *	47.00	13.6	36.20	47.80
		10^{-5}	6.60 *	28.60 *	42.00	11.4	34.00 *	42.00
		Control	9.20	38.40	46.40	11.6	37.00	43.60
		S.Em	1.18	1.73	5.49	1.64	2.30	2.65
		CD 5%	1.15	1.69	5.36	1.60	2.24	2.59

Table 1.2. Sporulation of *Trichoderma viride* as influenced by Nimyle and Well Guarddilution.

			Well Guard			Nimyle		
			Days of Incubation			Days of Incubation		
			2 Day	3 Day	4 Day	2 Day	3 Day	4 Day
(Treatment)	Sporulating Zone (Mean in mm ^{2})	**10^{-3}**	7.54 *	39.58 *	73.51*	38.37	114.98	123.78
		10^{-4}	23.88 *	94.88	153.94	47.75	123.15	140.11
		10^{-5}	23.45 *	87.34 *	131.95	37.07	114.98	139.49
		Control	28.90	105.56	143.8	38.33	114.98	157.08
		S.Em	5.95	17.25	18.71	7.22	8.32	0.11
		CD 5%	5.82	16.85	18.28	7.06	8.13	0.11

Table 1.3 Mycelial growth (mm) as influenced by Well Guard.

	P.F			H.U			C.I		
T	Inoculation Days			Inoculation Days			Inoculation Days		
	3	**8**	**9**		**3**	**8**	**9**		**3**
10^{-3}	5.80*	19.60 *	24.80 *	**10^{-3}**	5.80*	19.60 *	24.80 *	**10^{-3}**	5.80*
10^{-4}	6.40	26.60 *	30.60	**10^{-4}**	6.40	26.60 *	30.60	**10^{-4}**	6.40
10^{-5}	12.80#	31.20*	35.40*	**10^{-5}**	12.80#	31.20*	35.40*	**10^{-5}**	12.80#
Control	11.40	34.40	46.20	**Control**	11.40	34.40	46.20	**Control**	11.40
S.Em	1.81	3.23	2.99	**S.Em**	1.81	3.23	2.99	**S.Em**	1.81
CD 5%	1.77	3.16	2.93	**CD 5%**	1.77	3.16	2.93	**CD 5%**	1.77

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RESEARCH ARTICLE

Water Soluble Component Present in waste *Azolla pinnata* D.S. Mitch. and its Utilization for Soil Quality Improvement

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ABSTRACT

The concept of using aquatic plants for different purposes is receiving special attention nowadays. Azolla pinnata is a branched free floating aquatic fern. With the increasing demand in agriculture it has become important for us to increase the productivity by using various fertilizers. But with the dreadful use of these products the soil has been affected badly because of the depletion in the essential minerals of the soil. So to overcome this problem it has become important for all of us to use a different remedy for the production of various fertilizers. Of different fertilizers, liquid fertilizers are again a special class of fertilizers, hold very strong promise in protected cultivation. The liquid fertilizers, as special class of fertilizers provide an enormous possibility of accommodate nutrient use across critical growth stages, a mandatory for better nutrient-use-efficiency. Being readily water soluble components present in Azolla acts as soluble fertilizers help fertigation. So, an attempt has been taken to analyse the impact of water soluble component of Azolla pinnata on alteration of both physico-chemical and elemental content of soil. An attempts were taken to use the water soluble components of Azolla pinnata as a biofertilizer. The novelty of this work is the utilization of water soluble component in an environment friendly way. This research address the research gap by analyzing the Azolla pinnata as a water soluble fertilizer. In the present study it was found that the Azolla pinnata contains different useful elements which is major and minor element for plant nutrient. In the present study, water soluble component of dry Azolla pinnata was added to the garden soil and both initial and final physico-chemical parameters and elemental contents of soil were analyzed. It was observed that the soil which were treated with water soluble component of Azolla pinnata contained more nutrient than the normal garden soil. So water soluble

components of Azolla pinnata can be recommended as organic fertilizer which can fulfil the nutrient level of soil and enhance the soil fertility.

Keywords: water soluble component of Azolla pinnata, soil, Physico-chemical parameters, , Elemental content.

INTRODUCTION

India is poised to play a major role in increasing the utility of land water and other natural resources to compete with the increasing rate of population. Farmers today are faced with challenging of meeting and ever increasing demand for a white range of high quality and safe foods. Intensification of agriculture by irrigation and enhanced use of fertilizers may generate pollution by increased level of nutrients in underground and surface waters. By using bio-fertilizer which are made from natural sources increases the fertility of soil and also productivity of crop. Liquid fertilizer is a special kind of fertilizer that help in fertigation. Fertigation is the technique of supplying dissolved fertilizer to crop through an irrigation system. Small applications of soluble nutrients saves labour, reduces compaction in the field, thereby enhancing productivity. *Azolla pinnata* is one of the aquatic plants with high biomass and protein production which can be used as a fertilizer in agriculture [1]. Nutritive value of *Azolla pinnata* is well documented and promotes it as a good source of protein as it contains around 21-23% crude protein It is also found to contain essential minerals like Iron, Calcium, Magnesium, Potassium etc. and appreciable quantities of Vitamins A and Vitamin B-12 .[2] It is considered to be the most promising because of the ease of cultivation, minimal water for propagation, high productivity and good nutritive value [3, 4]. Nitrogen is the most limiting factor in crop production and it is essential for growth, protein manufacture and yield. *Azolla pinnata* fern is prevalent worldwide and has been used over centuries for fertilization in paddies as a source of nitrogen. By *Azolla pinnata* nitrogen fixation occure which enhance the growth of plants. Thus, use of water soluble fertilizer such as *Azolla pinnata* is a good alternative to inorganic fertilizers. The organic residue produced from any plants or animal origin has play important role in changing soil quality. The organic material affect the soil physically [5], soil nutrient content and faunal diversity of soil [6]. As we know that bio-fertilizers are the major source to enhance the growth and development of plants, So in this study water soluble fertilizer from *Azolla pinnata* was analyzed and physico-chemical parameters of both garden soil and garden soil treated with water soluble component of *Azolla pinnata* was compared for knowing either that is beneficial or harmful for environment.

MATERIALS AND METHODOLOGY

In this study, soil samples were collected from a garden of Centurion University of Technology and Management, BBSR, Odisha, at depths of 18 cm using soil auger. The samples were collected in a polyethylene bags and properly labelled. Then the collected samples were taken to the laboratory and treatment was done for the preservation of soil and further analysis has been done as per standard procedure[7]. The collected samples were air dried in sun light for about twenty four hour. Then the samples were dried in an oven at 105˚C till complete dehydration. Then the sample was ground in a mortar pestle then passed through 0.5 mm nylon mesh sieve. These soil samples were again packed with the complete labelling and preserved for further analysis. *Azolla pinnata* were collected from botanical garden of Centurion University of Technology and Management, Bhubaneswar, Odisha. The physico-chemical parameters like pH, E.C., soil moisture percent (%), water holding capacity of soil and elemental content of both soil and water soluble component of *Azolla pinnata* were analyzed using standard methods.

STATISTICAL ANALYSIS AND PRESENTATION OF DATA

All the experiments were done in triplicates and the data presented in the figures are the means of three independent experiments. The data were analyzed statistically and standard errors of mean (SEM) were given wherever required.

RESULTS AND DISCUSSION

Physico-chemical parameters of elemental analysis of soil: The physico-chemical parameters like pH, Electrical conductivity (E.C), soil moisture content (%), water holding capacity (W.H.C), and different elements/compound contents present in garden soil and garden soil treated with water soluble component of *Azolla pinnata* were analysed.

pH: The pH values of the soil sample collected from our college garden area was found within 7.6 to 7.8. So the soil sample was considered to be basic. After addition of water soluble component of *Azolla pinnata* it was found to be 6.8 to 7.2 which indicates that the water soluble component of *Azolla pinnata* neutralizes the alkaline soil. Then after addition of water soluble component of *Azolla pinnata* it was found to be decreased.

Electrical conductivity (E.C): The conductivity values in the soil samples of the area under study were found to range from0.813 mho/cm to 0.822 mho/cm. After addition of water soluble component of *Azolla pinnata* it was found to be 0.892mho/cm to 0.971mho/cm. Then, after addition of *Azolla pinnata* soluble component it was found to be increased.

Soil moisture content: At pre-monsoon period moisture content were found in the range of 8.0% to 10.2% whereas at post-monsoon period it was ranged from 10.0% to 11.7.0%, which indicated that the moisture content present in soil of the area is suitable for crop production. After addition of water soluble component of *Azolla pinnata* it was found to be increased that is from 12% to 14% .

Water holding capacity (W.H.C): Soil water holding capacity is a term that all farms should know to optimize crop production. When there is a difficult in the amount water in the soil, the soil profile needs to be replenished by precipitation or irrigation. In the study the soil had range between 156.55 to 158.58. After addition of water soluble component of *Azolla pinnata* it was found to be 159.19 to 162.16. After addition of water soluble component of *Azolla pinnata* it was found to be increased.

Elements/compound contents: In this study, elemental analysis of soil had been done in the basis of XRF (X-ray fluorescence). The soil was found to be contained many elements/compounds i.e given in table. There are several elements and compounds were found to be present in water soluble component of *Azolla pinnata* which enhanced the nutrient level of garden soil. After addition of water soluble component, concentration of different valuable elements like P_2O_5, SO_3, Cl, K_2O, CaO and Rb_2O were found to be increased which enhanced the soil nutrient level. In a study it was reported that the application of egg shell waste enhances the soil fertility [8]. In another study, it was reported the application of compost act as fertilizer on growth of onion, on barley. From another experiment, it was found that, the tea dust waste compost are highly desirable for plant growth [9], it was also found that *Azolla pinnata* is beneficial to wheat when applied in a rotating rice-wheat cropping system [10]. The presence of some metals like copper, zinc, iron, manganese, molybdenum and nickel are essential micronutrient for plant growth [11]. Similarly, small amount of different metals enhance the plant growth like nickel in *Macrotyloma uniflorum* [12]. Compost prepared from organic waste [13] increases soil organic matter on land [14] and provide plant nutrients in slowly available form [15]. Similar results were also reported in growth of peanut crops grown with water soluble component of *Azolla pinnata* treated soil [16].

CONCLUSION

Azollla pinnata can be used as water soluble fertilizer due to presence different valuable macro and micro nutrient for plants. In the present study , it was found that the water soluble component treated soil contains much more nutrient than the normal garden soil. So this research can say that water soluble component of *Azolla pinnata* can fulfil the

mineral requirement for the plants growth. Overall it is an excellent organic manure for plants. It can be recommended for utilization at crop field for better growth and development of plant without causing any harm to the plant as well as soil.

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Table-1: Comparison between garden soil and garden soil treated with water soluble component of *azolla pinnata*

Parameters	Unit	Garden soil	Garden soil treated with water soluble component of *azolla pinnata*
pH		7.6 ± 0.067	6.98 ± 0.14
Electrical conductivity	mho/cm	0.813 ± 0.051	0.892 ± 0.072
Water holding capacity	ml/kg	156.55 ± 0.51	159.19 ± 0.43
Moisture Content	%	10.2 ± 0.58	12 ± 0.86

Values of four replicates ± SEM

Table-2:Comparison between the elemental content present in garden soil, water soluble component of *azolla pinnata* and garden soil mixed with tea water soluble component of *azolla pinnata*

Elements/Compound	Unit	Elemental Content		
		Garden Soil	Water soluble component of *Azolla pinnata*	Garden soil + water soluble component of *Azolla pinnata*
Al_2O_3	%	10.713 ± 0.635	0.4745± 0.0855	10.291± 0.088
SiO_2	%	46.183 ± 0.601	3.081± 0.062	42.309± 0.242
P_2O_5	%	1.033 ± 0.001	3.1215± 0.0905	1.112± 0.024
SO_3	%	1.24 ± 0.002	3.86± 0.012	1.342± 0.034
Cl	%	2.923 ± 0.243	35.376± 0.559	1.286± 0.026
K_2O	%	1.45 ± 0.053	29.7405± 0.7485	2.113± 0.0118
CaO	%	0.133 ± 0.004	18.8725± 0.4535	1.118± 0.024
TiO_2	%	2.933 ± 0.233	0.1555± 0.0105	2.752± 0.028
V_2O_5	%	0.133 ± 0.002	00± 00	0.098± 0.026
ZrO_2	%	37.123 ± 0.321	00± 00	30.121± 0.022
MnO	Ppm	514.321 ± 2.620	2.807± 0.446	506.308± 0.284
Fe_2O_3	Ppm	336.231± 0.313	2.095± 0.149	332.212± 0.364
NiO	ppm	188.703± 1.583	119.3± 5	195.824± 0.086
Cr_2O_3	ppm	350.525± 2.292	63.7± 25.6	334.022± 0.828
CuO	ppm	74.312 ± 0.297	156.95± 4.75	70.686± 0.064
ZnO	ppm	100.211± 0.573	727.15± 17.05	98.642± 0.083
Ga_2O_3	ppm	146.903± 0.607	00± 00	140.464± 0.044
As_2O_3	ppm	31.208± 0.289	00± 00	28.008± 0.062
Rb_2O	ppm	12.103± 0.347	123.7± 1.1	121.514± 0.124
SrO	ppm	137.209± 0.636	82.85± 1.65	167.083± 0.086
Y_2O_3	ppm	131.713± 0.285	00± 00	52.001 ± 0.072
Nb_2O_5	ppm	31.025± 0.573	00± 00	29.122 ± 0.044
SnO_2	ppm	96.002± 2.092	00 ± 00	89.124 ± 0.082

Values of five replicates ± SEM

AUTHOR

Dr. Atia Arzoo is educated in Utkal University, Bhubaneswar, Odisha. Her areas of research and consulting interest include environmental pollution control and management especially in the field of Phytoremediation and waste management. Prior to joining Centurion University of Technology and management, she was working as guest faculty to Utkal University. She is having teaching experience of 2 years. She has published 20 research papers in different national and international journals. She has guided 6 M.Sc. students for pursuing their dissertation project and now, she is guiding 4 M.Sc. students and 1 Ph.D. student. Now she works as the Head of the department, Department of Applied chemistry and Environmental Science.

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RESEARCH ARTICLE

Comparative Studies on Biocontrol of Noxious Weed *Parthenium hysterophorus* L. by Application of *Eucalyptus globulus* Labill. and *Hyptis suavolence* L.

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ABSTRACT

Parthenium hysterophorus L. is considered as one of the harmful weeds because of its invasiveness, rapid multiplication rate and adverse impacts on environment and human health. The novelty of this work is to manage the weeds by employing organic matters instead of harmful chemical weedicides which have an adverse environmental impacts due to accumulation in soil and leaching to water bodies. Researchers have studied the allellopathy impact of both the plants, However there is little report available on the use of this extract as natural herbicide. This study was carried out to assess the allellopathic effect of the aqueous extract of leaves of *Eucalyptus globulus* Labill. and *Hyptis suavolence* L. on the control of noxious weed *Parthenium historephorus* L. The extracts of both the leaves were used in same concentration (00 % - 100%) and their impact on seed germination and growth of seedlings were observed. The results obtained from utilizing *Eucalyptus globulus* Labill. extract showed more effective in terms of germination, seedling growth, seedling vigour indices and tolerance indices in comparison with *Hyptis suavolence* L. leaf extract. The experiment also showed complete inhibition in germination of seed. The current study gives an idea about the use of organic products from plants considered as better alternatives to harmful synthetic herbicides which is the eco-friendly way to biocontrol the weeds to reduce environmental pollution.

Key words: Biocontrol, Parthenium, Allelopathy, Eucalyptus, Hyptis

INTRODUCTION

Weeds are an important issue which influence the production of crop through competition for availing nutrition from environmental resources and cause productivity loss [1]. Weeds are also responsible for degradation of environment in terms of threatened the biodiversity [2]. *Parthenium histerophorus* L. is one of the harmful and allergy causing weeds which is resistant to traditional methods of weed management due to its invasiveness and rapid spreading potential. *Parthenium hysterophorus* L. has spread in land area about 35 million hectares in India [3]. As *Parthenium hysterophorus* L. affects natural ecosystem like agriculture, human and animal health so it is the need of the day to find out the management options for *Parthenium hysterophorus* L.. There is ever-increasing interest globally for reducing the use of synthetic herbicides in the all sectors to reduce the herbicide level in human diet [4]. This weed has been managed by continous use of chemical herbicides by which causes environmental pollution is much more. There is another approach like allelopathy is an eco-friendly and a viable option. Allellopathy is the beneficial or harmful effects of one plant parts on another through the liberation of certain chemicals into its surroundings [5]. The allelochemicals affect in crop/weed by interactions for availing nutrients [6]. Application of allello-chemicals is an actively precious and sustainable management process managing weeds. *Eucalyptus globulus* Labill. is important tree species, which are extensively spreads in tropics and subtropics region shows allellopathy potential. Another species *Hyptis suavolence* L. is also having the property of allellopathy potential [7].

The use of herbicides globally is approximately 48 % of the total output of different pesticides like herbicide, fungicide and insecticide [8]. China produced herbicide approximately 1.77 million tons which is the 55 % of total output of different pesticides used in agriculture [9]. Hence a comparative study was undertaken to study the allellopathic potential of aquous leaf extract of Eucalyptus and *Hyptis suavolence* L. on controlling *Parthenium hysterophorus* L. Current research is focused on the weed management by using an effective biocontrol method by using plant extracts as an ecofriendly and cost effective alternative for replacement of synthetic weedicides in weeds management. The present study is aim to explore the use of plant extracts as one of the future solutions for the use of a natural, cost effective and eco-friendly approach for an effective alternative in the weed management like *Parthenium hysterophorus* L..

MATERIALS AND METHODS

Seeds of *Parthenium hysterophorus* L. were collected from road sides and near agricultural fields of Khordha district, Odisha where the plants grown densely. The seeds which were healthy and free from pathological conditions were collected and repeatedly washed in tap water to remove adsorbed dust particles. The seeds were left for one day and then soaked the water by using tissue paper until dry and then kept in a plastic container for further use. For allelopathy study, two allelopathic plants: *Eucalyptus globulus* Labill. and *Hyptis suavolence* L. were selected for the preparation of extract. Stock solution of aqueous leachates of selected plants were prepared by using distilled water (1:10 w/v) for 24 hours and filtered the aquous extract by using Whattman No.1 filter paper. This stock extract was diluted with distilled water to prepare required concentration (00% to 100%) of leachate. Four replicates of each 50 healthy seeds of *Parthenium hysterophorus* L. were placed on extracted treated germination paper in properly sterilized petridishes. The petridishes were maintained at 26°C and 94 % humidity with exposure to 20 ml of different concentration of aqueous leachates of extract and distilled water for comparison as control.

Percentage of germination (G %) was calculated by the formula [10].

$$G\,\% = \frac{\text{Total no. of seed germinated}}{\text{Total no.of seed tested}} \times 100$$

The percentage of phytotoxicity of the was calculated by the formulae suggested by Chou et. al (1978) [11].

$$\text{Phytotoxicity (\%)} = \frac{\text{Radicle length of control} - \text{Radicle length of test}}{\text{Radicle length of control}} \times 100$$

According to Baki and Anderson (1973) [12] Seedling vigour indices (SVI) were calculated by using the formulae:
SVI = Germination percentage × Radicle length

According to Turner and Marshal (1972) [13], The tolerance indices (TI) of the seedlings were calculated by using the formula:

$$TI = \frac{\text{Radicle length of seed intest}}{\text{Radicle length of control}} \times 100$$

STATISTICAL ANALYSIS

The statistical implication of various paremeters were studied utilizing one way Annova by MS-Excel. The p-value less than 0.05 implies significant contributions.

RESULTS AND DISCUSSION

The effect of leaf extract of both *Eucalyptus globulus* Labill. and *Hyptis suavolence* L. showed that the percentage of germination was significantly decreased with increasing concentration of leachate. Similarly the radicle length of the seedling were also found to be decreased significantly with increasing concentration of leachate of both the extract. The other paremeters like Seedling vigour indices and tolerance indices was also found to be decreased whereas the level of phytotoxicity was found to be increased with increasing leachate concentration of both the leaf extract. But the *Eucalyptus globules* Labill. leaf extract showed better result in comparison with hyptis leaf extract. The data of the present study are presented in table-1 and 2. The results were in argument with the findings of a research [14 & 15] that the aquous extract of different plant showed a negative effect on the seed germination and seedling growth of all weeds studied. In another study, reduction in seedling growth was also reported under allellopathy stress [16 & 17]. Similar result on the growth of tomato, radish, cucumber and banyard grass was found with the application of *Lantana camara* extract [18]. Based on the presented research results, it was found that the use of the leaves of both plant species are alternative to using weedicides to control *Parthenium hysterophorus* L. but *Eucalyptus globulus* Labill. was found to be more effective than the *Hyptis suavolence* L.

CONCLUSION

The aqueous extract of *Eucalyptus globulus* Labill. leaves produced better inhibiting effect than the *Hyptis suavolence* L. leaves on seed germination and seedling growth, hence the *Eucalyptus globules* Labill. leaves extract can be used in eco-friendly, cost effective and bio-control method for weed management like *Parthenium hysterophorus* L.. More future studies are required to find the inducing agents which are responsible for these inhibition of germination.

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Table-1: Impacts of two different extract on germination of Parthenium seeds.

	Germination (%)		Radicle length (cm)	
Conc. of extract (From stock of 1:10 w/v)	**Eucalyptus extract**	**Hyptis extract**	**Eucalyptus extract**	**Hyptis extract**
Control (00 %)	82.5 ± 2.380	83.5±1.201	4.85 ± 0.238	4.925 ± 0.275
20 %	52.25± 2.217	56.25±1.5	4.025 ± 0.695	4.4 ± 0.283
40 %	24.25±1.5	24.25 ± 1.708	3 ± 0.365	3.5 ± 0.115

60 %	9.75±0.957	11 ± 1.633	2.325 ± 0.309	2.675 ± 0.171
80 %	2.75 ±0.957	3.25 ± 0.957	1.475 ± 0.499	1.725 ± 0.096
100 %	0.75 ±0.957	1.25 ± 0.957	0.3 ± 0.476	0.525 ± 0.512
	*0.038	*0.046	*0.003	*0.003

Values of four replicates ± SD
*indicates the p-values

Table - 2: Impact of different concentration of aquous Eucalyptus extract on seedling vigour indices (SVI), tolerance indices (TI) and percentage of phytotoxicity.

Conc. of extract (From stock of 1:10 w/v)	Seedling Vigour Indives		Tolerance Indices		Percentage of phyto-toxicity	
	Eucalyptus extract	Hyptis extract	Eucalyptus extract	Hyptis extract	Eucalyptus extract	Hyptis extract
Control (00 %)	400.125	411.237	100	100	00	00
20 %	210.306	247.5	82.989	89.340	17.01	10.660
40 %	72.75	84.875	61.855	71.066	38.144	28.934
60 %	22.668	29.425	47.938	54.315	52.062	45.685
80 %	4.056	5.606	30.412	35.025	69.587	64.974
100 %	0.225	0.656	6.185	10.660	93.814	89.340

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RESEARCH ARTICLE

Studies on the Changes in Various Water Quality Parameters Due to Coal Mining at Talcher Mining Areas of Odisha, India

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ABSTRACT

Odisha is a state of India which is well known for production of mineral resources including metallic, non metallic and fuels. In a mining area, ecological disturbance occurs due to deposition of different types of pollutants during excavation and extraction of mineral ores. Presently, water bodies of the Talcher colliery areas are being contaminated with the hazardous pollutants discharged into it by the mines' waste waters, which pose a constant threat to the human health and live-stock. This study aims to assess the impact of colliery pollutants generated from different coal mines of Talcher mining area on nearby water bodies including both surface water as well as ground water. In this study, water samples were collected from different sources of surface water as well as ground water present in and around Talcher colliery areas. Different physico-chemical parameters such as pH, Electrical conductivity, Total dissolved solids, Total suspended solids, Total hardness, Total alkalinity, Calcium, Magnesium, Fluoride, Chloride, Iron, Total Chromium and Total Nickel content of water were analysed. The results of this investigation indicated that the migration of colliery pollutant leads to hydrological pollution with increasing level of total dissolved solids, fluoride concentration and also some heavy metal pollutants like iron and chromium which leads to health hazards of both plants and animals.

Keywords: Coal mining, Physico-chemicals parameters, Water, Odisha

INTRODUCTION

Odisha is a state of India has huge mineral resources and also produces enormous minerals including non-metallic, metallic and fuel minerals. Odisha state has two coalfields i.e. Ib-River Coalfield and Talcher Coalfield. In mining areas, some ecological disturbances always occur which is induced by mined-out region. Heavy metals occur in the soil in soluble form and in combined state. However, only soluble, exchangeable and chelated metal species in soils are mobile and hence more available in water [1].

Water is essential for life but it transmits diseases in plants and animals. Many of the people are exposed to unsafe level of chemical contaminants in their drinking water [2]. Water in its natural state may not be pure since it is a universal solvent with the ability to dissolve numerous chemicals and thus carry a lot of impurities that can be injurious to health if it exceeds tolerance limit [3]. The natural quality can vary from one rock type to another and also within aquifers along its flow paths. There is also possibility for chemical reactions between the water and rock material through which its flow depending on the flow path [4]. According to [5] and National academy of science [6] over one billion people lack access to clean and safe water. The available fresh water to man is hardly 0.3-0.5% of the total water available on the earth [7]. Many people in the world especially majority of which live in rural areas among the poorest and most vulnerable do not have access to safe and clean drinking water [8]. Therefore, it is necessary to identify the hazardous pollutants and remove it from the polluted places. The present investigation was undertaken to estimate the changes in various water quality parameters due to coal mining at Talcher mining areas of Odisha, and to check either it is suitable for human health or not.

MATERIALS AND METHODS

Geographical location of the Study area: Talcher coalfield constitutes the south eastern part of the Lower Gondwana Mahanadi Master Basin and occupies an area of over 1813 sq. km. The coalfield is in between 20°50' and 21°15' N latitude and 84°09' and 85°33' E longitudes and is mainly consists of the Brahmani River Valley. It covers Dhenkanal and Angul districts along with a small portion of adjoining Sambalpur district of Odisha. For the present study, ten water sources were selected namely (i) Talabera village (well water), (ii) Rakas village (well water), (iii) Hensmul village (well water), (iv) Dera village (tube well water), (v) Jilinda village (well water), (vi) Naraharipur village (pond water), (vii) Old quarry at Jagannath colliery area, (viii) Mine discharge water at confluence with Bangarunala, (ix)Mine discharge water at Jagannath Colliery and (x) Pond water near Bharatpur Colliery. These water bodies are surrounded by mining pockets, human settlements, some industries and agricultural fields. Some of these sites had received partially treated effluent from the mining units located near to it.

Collection of water samples: Water samples were collected from different sampling sites; surface water collected from nearby streams, rivers, ponds and quarries while ground water collected from nearby wells and tube wells. Composite water samples were collected from the all ten water sources in pre-sterilized plastic cans/bottles according to standard methods of [9]. Representative water samples were analysed for different physico-chemical parameters as well as pollutants concentrations in School of Applied Sciences, Centurion University of Technology and Management, Odisha.

Analysis of physico-chemical parameters: The standard methods were followed for analyzing physico-chemical parameters and metal contents (total chromium, total nickel and total iron) in water. The analyses of different parameters of water were made by standard methods recommended by [9] and [10]. Temperature and pH were measured at sampling sites with the help of digital portable kit. All the collected samples were brought to the laboratory and stored at 5 ± 1 °C and analysis of various parameters following standard methods.

RESULTS AND DISCUSSION

Results of analysis of different physico-chemical parameters of ground and surface water samples of selected sites of Talcher colliery area are presented in Table 1 & Table 2.

pH: The pH values in ground water as well as surface water were found mostly confined within the range of 6.0 to 8.1. The pH values of most of the samples are well within the limit prescribed by [11] for various uses of water including drinking and other domestic supplies.

Electrical Conductivity: The measurement of electrical conductivity is directly related to the concentration of ionized substance in water and may also be related to problems of excessive hardness or other mineral contaminants. The conductivity values in both surface and the ground water samples were found to range from 360 μS/cm to 980 μS/cm.

Total dissolved solid: In natural water dissolved solids consists mainly of inorganic salts such as carbonates, bicarbonates, chlorides, sulphates and nitrates of calcium, magnesium, sodium, potassium, iron etc. and a small amount of organic matter and dissolved gases. In the present study the values of total dissolved solids (TDS) in the ground water were in the range of 232 mg/L. to 584 mg/L and surface water ranged from 384 to 648 mg/L.

Only one ground water sample and three surface water samples were found above the desirable limit of 500 mg/L but well within the maximum permissible limit of 2000 mg/L (Table 2 & Table 3). The TDS content at ground water was comparatively lower than the surface water which might be due to more mineralization of surface water as compared to the ground water. Water containing more than 500mg/L of TDS is not considered desirable for drinking water supplies, though more highly mineralized water is also used where better water is not available. For this reason, 500 mg/L is accepted as the desirable limit while 2000 mg/L as the maximum permissible limit has been suggested for drinking water [11]. However, it is reported that water containing TDS more than 500mg/L caused gastro-intestinal irritation [11].

Alkalinity: The presence of carbonates, bicarbonates and hydroxides are the main cause of alkalinity in natural waters. Bicarbonates represent the major form since they are formed in considerable amount from the action of carbonates upon the basic materials in the soil. In the study sites the alkalinity value in ground water was varied from 148 mg/L to 282 mg/L while in surface water from 216 mg/L to 394 mg/L. The alkalinity level of three ground water samples and all surface water samples were found crossed the desirable limit of 200 mg/L but are within the maximum permissible limit of 600 mg/L. The high alkalinity value at some locations may be due to the action of carbonates upon the basic materials in the soil.

Total hardness: The total hardness is the sum of concentration of alkaline earth metal cations present in the water. It is due to presence of Calcium and Magnesium ion in water [12]. Calcium and Magnesium along with their carbonates, sulphates and chlorides make a water hard. A limit of 300 mg/L has been recommended for potable water. The total hardness of the collected water samples in the study area were within the range of 83 mg/L to 306 mg/L. As evident from the results no ground water sample and one surface water sample had exceeded the desirable limit of 300 mg/L but not crossed the maximum permissible limit of 600mg/L.

Calcium hardness: Calcium hardness is an important component of the carbonic buffer system. It is also cycle through biotic and abiotic components of the ecosystems. Calcium hardness originates from natural processes is a dissolvent of minerals which contains calcium and other sources such as industrial wastes and agricultural wastes but found nontoxic. The desirable limit for calcium is 75 mg/L [11]. In the study area the values of calcium in ground water were estimated to vary from 38 mg/L to 85 mg/L and in surface water from 56 mg/L to 99 mg/L.

Magnesium hardness: Magnesium hardness is an important component of total hardness, which originates from different processes such as mining activities, degradation of rocks etc. It is also cycled through biotic and abiotic components of the ecosystems. The desirable limit for magnesium is 30 mg/L [11]. In the study area the values of magnesium in ground water were varied from 11 mg/L to 27 mg/L and in surface water ranged from 18 mg/L to 51 mg/L.

Chloride: The chloride content in water of the study area was quite low and varies from 14 to 65mg/L. No sample in the study area had crossed the desirable limit of 250 mg/L [11]. The limits of chloride have been laid down primarily from taste considerations.

Fluoride: The fluoride content in water of the study area was found within the range of 0.1 mg/L to 2.1 mg/L. However, two surface water samples in the study area were found crossed the desirable limit of 1.5 mg/L [11].

Sulphate: The sulphate content in water generally occurs as soluble salts of calcium, magnesium and sodium. The content of sulphate changes significantly with time during infiltration of rainfall and ground water recharge, which mostly takes place from stagnant water pools and surface runoff water collected in low laying areas. The concentration of sulphate in the study area varied from 31 mg/L to 147 mg/L in all the samples falling within the desirable limit of 200 mg/L.

Nitrate: Nitrate content in drinking water is considered important for its adverse health effects. The occurrence of high levels of nitrate in ground water is a prominent problem in many parts of the country. The nitrate content of water in Talcher area varied from 4 mg/L to 43 mg/L in all samples falling within the desirable limit of 45 mg/L [11]. A nitrate is an effective plant nutrient and is moderately toxic. Its concentration above 45mg/L may prove detrimental to human health. In higher concentrations, nitrate may produce a disease known as methanoglobinemia (blue babies) which generally affects bottle-fed infant, repeated heavy doses of nitrate on ingestion may also cause carcinogenic effect.

Heavy metals: The contamination of ground water by heavy metals has received enormous attention during recent years due to their toxicity and accumulative behaviour. These elements contrary to most pollutants are not biodegradable and undergo a global eco-biological cycle in which natural water are the main pathway.

Chromium (Cr): The maximum permissible limit for Cr in water is 0.1 mg/l. The values of Cr in four samples out of 10 were found within the desirable limits.

Iron (Fe): The desirable limit for iron in water is 0.3 mg/l. Iron has been considered to be an essential trace element for human and animal health. In the present study one ground water sample and two surface water samples were found to cross the desirable limit of 0.3 mg/l.

Nickel (Ni): The maximum permissible limit for Ni in water is 0.2 mg/l. Nickel has been considered to be an essential trace element for human and animal health. In living systems, it is associated with DNA and RNA molecules and also a regulatory element for the various enzyme systems [13]. It causes blindness both in human and animals, increased blood sugar level and serum cholesterol as well as local necroses in the liver tissue. Drinking water and food are the main sources of exposure for the general population with the average American diet containing about 300 µg Ni/d. In this present study the values of nickel in all water samples were below detectable limit of 0.01mg/L.

CONCLUSION

Water resources are often considered to play a vital role in ensuring social and economic development. The pace of urbanization and other anthropogenic activities including mining around the water bodies impose severe problems to physico-chemical environment of the water resource and the health of the ecosystem is deteriorating. The results showed that pH of all the samples of surface and ground water was within the permissible limits, whereas values of total dissolved solids, total hardness, fluoride content and some heavy metal contents like chromium and iron were found to be relatively higher than the desirable limits. Almost all the samples were found to be enriched with the selected toxic metals, whereas the concentration of nickel was found within the permissible limits. The concentration of selected toxic metals in the waste water of the study area, being used for the irrigation purpose, was found to be satisfactory but not suitable for drinking purposes.

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Table-1: Different sampling sites in and around Talcher Coal mining area.

Sl. No	Sampling Site	Sample Type
1	Talabera village (well water)	Ground water
2	Rakas village (well water)	Ground water
3	Hensmul village (well water)	Ground water
4	Dera village (tube well water)	Ground water
5	Jilinda village (well water)	Ground water
6	Naraharipur village (pond water)	Surface water
7	Old quarry at Jagannath colliery area	Surface water
8	Mine discharge water at confluence with Bangarunala	Surface water
9	Mine discharge water at Jagannath Colliery	Surface water
10	Pond water near Bharatpur Colliery	Surface water

Table-2: Different physico-chemical parameters of ground water samples of selected sites of Talcher Coal mining area.

Sl. No.	Parameters	Unit	Desirable Limit	Sampling sites				
				S1	S2	S3	S4	S5
1	pH	_	6.5-8.5	8.1±0.114	8.3±0.084	7.9±0.126	8.2±0.092	7.8±0.084
2	Electrical conductivity	µs/cm		630.3±1.55	585.2±1.65	668.5±2.02	957.3±2.01	618.6±1.65
3	Total dissolved solids	mg/L	500	416±2.12	398±1.66	468±2.01	584±1.45	365±1.55
4	Total alkalinity	mg/L	200	193±1.06	282±0.84	185±1.22	208±0.96	148±1.04
5	Total hardness	mg/L	300	116.1±1.24	180.2±1.08	156.2±0.98	184.1±1.05	118.3±1.21
6	Calcium hardness	mg/L	75	64.2±0.86	71.2±0.41	54.2±0.76	84.5±0.48	42.2±0.86
7	Magnesium hardness	mg/L	30	12.6±0.42	26.5±0.68	24.8±0.12	24.2±0.09	18.5±0.26
8	Chloride	mg/L	250	32.6±0.13	38.4±0.24	42.4±0.11	78±0.26	46.6±0.28
9	Fluoride	mg/L	1.5	1.2±0.08	0.47±0.01	0.18±0.03	1.4±0.06	0.52±0.02
10	Sulphate	mg/L	200	66.4±1.08	64.8±1.24	78.4±0.66	114±0.98	52±0.54
11	Nitrate	mg/L	45	12.8±0.02	26.4±0.24	22.6±0.26	32.2±0.38	28.5±0.08
12	Total chromium	mg/L	0.1	<0.001	0.08±0.01	<0.01	0.07±0.01	<0.01
13	Total iron	mg/L	0.3	<0.001	<0.01	0.28±0.02	0.34±0.01	0.18±0.01
14	Total nickel	mg/L	0.02	<0.001	<0.01	<0.01	<0.01	<0.01

Values of five replicate ± SEM

Table-3: Different physic-chemical parameters of surface water samples of selected sites of Talcher Coal mining area.

Sl. No.	Parameters	Unit	Desirable Limit	Sampling sites				
				S6	S7	S8	S9	S10
1	pH	_	6.5-8.5	8.4±0.12	8.2±0.09	8.3±0.08	8.2±0.11	8.4±0.08
2	Electrical conductivity	µs/cm		393.2±1.65	938±2.03	911±2.02	553±1.65	936±1.55
3	Total dissolved solids	mg/L	500	232±1.26	562±1.49	592.5±1.86	384±1.42	648±1.08
4	Total alkalinity	mg/L	200	218±1.64	216±1.28	232.5±1.42	268.2±1.08	394.2±1.24
5	Total hardness	mg/L	300	83.3±0.96	305.2±1.28	170.6±1.06	131.5±0.84	181.6±0.78
6	Calcium hardness	mg/L	75	38±0.12	98.2±0.46	68.4±0.62	56.8±0.76	72.6±0.18
7	Magnesium hardness	mg/L	30	11±0.08	50.3±0.15	24.6±0.12	18.4±0.06	26.5±0.16

8	Chloride	mg/L	250	14±0.06	64.5±0.04	40.2±1.08	46.4±1.21	64.6±1.46
9	Fluoride	mg/L	1.5	0.14±0.03	2.1±0.02	0.8±0.02	1.4±0.04	1.6±0.03
10	Sulphate	mg/L	200	31±0.08	146.2±0.23	112.5±0.16	98.6±0.11	86.8±0.08
11	Nitrate	mg/L	45	4.2±0.01	42.8±0.84	32.6±0.23	28.4±0.06	32.6±0.12
12	Total chromium	mg/L	0.1	<0.01	0.08±0.01	<0.01	0.04±0.01	<0.01
13	Total iron	mg/L	0.3	<0.01	0.32±0.02	0.16±0.01	0.08±0.01	0.32±0.01
14	Total nickel	mg/L	0.02	<0.01	<0.01	<0.01	<0.01	<0.01

Values of five replicate ± SEM

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RESEARCH ARTICLE

Impact of Certain Macro-Economic Indicators on Ownership of Room Air-Conditioners across Indian States

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ABSTRACT

A number of organizations that include consulting firms, brokerage firms, and government agencies often make forecast for sales of different products and services at industry level. Such publicly available forecasts along with data on past trends could be good starting point for sales departments to make forecast for their own company at different geographic levels. Machine Learning implemented through Artificial Neural Network method has emerged as an easier and popular approach to estimate future demands. This article takes data from two freely available sources on certain macro-economic indicators like Gross State Domestic Product, Growth Rate, Per Capita Income, and Total number of Households for eighteen states and two union territories of India and analyses their impact on AC ownership across these states using Artificial Neural Network method.

Keywords: Demand and sales forecasting, macro-economic indicators, Gross State Domestic Product, Growth Rate, Per Capita Income, Total number of Households.Machine Learning, Artificial Neural Network

INTRODUCTION

Background of the Study: Many consulting firms like pwc, and McKinsey, brokerage firms like Motilal Oswal and Edelweiss, and non-profits like India Brand Equity Foundation (IBEF), a Trust established by the Department of Commerce, Ministry of Commerce and Industry, Government of India, come out with demand forecasts for various industries from time to time. These reports are often available for free and are useful as starting points for sales forecasting using judgemental methods at individual firm level. However, due to the simple methodologies used in

the research behind these reports, the forecasts given by them should be used along with suitable statistical methods to improve the accuracy of the forecast. Artificial Neural Network is one such method that has gained popularity in recent years (Zhang 2004). This article takes data from one such publicly available data on the room air conditioner (AC) market in India (Oswal 2018) and certain macro-economic data on some Indian states (ESOPB 2020) to find if the variation in AC ownership across states has any relationship with the variations in the select macro-economic indicators. The Oswal (2018) report assumes that 'household owning refrigerators but not AC' and 'households owning washing machines but not AC' are potential customers for ACs. Though this assumption may seem tempting for the marketers, it may be fallacious.

This article looks into the impact of four select macro-economic indicators - Gross State Domestic Product (GSDP), Growth Rate (GR), Per Capita Income (PCI), and Total number of Households (TH) across eighteen states and two union territories in India, on AC ownerships (predicted AC sales PAC)

LITERATURE REVIEW

Demand and Sales Forecasting: Sales forecasting involves predicting the quantity of a product or service target customers will buy, given a marketing-mix program in a given time period moderated by the market conditions. Accurate sales forecasting is important for any business entity for its planning at various levels (Armstrong 2008, Mentzer and Moon 2004, Efendigil, Önüt and Kahraman 2009, Chintagunta & Nair, 2011). Though lot of progress has been made in the forecasting techniques over the last few decades, business entities are yet to derive benefit from them as many of them rely on basic techniques and spread sheets (Canitz, 2016). The large number of available forecasting methods derive broadly from two sources – Judgemental and Statistical. Armstrong (2008) summarizes those methods and their interrelationships in Figure 1.

Organizations and their sales teams often use various Judgemental methods as they are perceived to be easier to use. However, there has been an increasing trend to integrate both the judgemental and the statistical methods (E.g., see Armstrong and Collopy 1998, Davydenko 2012, Bunn and Wright 1991, Webby and O'Conner 1996). Judgmental forecasts generally add contextual information for the final forecast. Given the right integration method, judgmental forecasts improve accuracy of the statistical forecast by proving additional information and the domain knowledge of the experts (Armstrong and Collopy 1998). However, as has been cited above, organizations often are not able to take the benefit of the advanced forecasting methods not because of judgemental methods, but because of the complexities of the statistical methods for them. For many of them, the Judgmental methods are often the primary forecasting tools. Rarely any one forecasting method will give a reliable estimate of future demands. It is advisable to use a number of judgemental and statistical methods and integrate the findings to improve the accuracy and reliability of the final forecast.

Use of Machine Learning in Demand & Sales Forecasting: Traditional statistical forecasting methods use time series data with the assumption that future demand can be estimated from past data statistically. This assumption may hold true in stable business environment, which is rarity. Many exogenous factors, which were not present in the past, could potentially influence future demand. To overcome this limitation, causal modelling methods have been proposed which work with such exogenous factors as macro-economic indicators, competitive strategies, natural forces etc (Chopra and Meindl2013). Cadavid, Lamouri and Grabot (2018) have argued that since Machine Learning can take different types of data and variables such as categorical variables, fuzzy variables, time series, text, image and other types of data, it can be said of providing causal modelling. Researchers have used machine learning for demand and sales forecasting through Artificial Neural Networks (ANN) for the last four decades for a variety of products and services (Cadavid, Lamouri and Grabot (2018).

With the increasing availability of software that use such advanced techniques as Artificial Neural Network (ANN), it has become easier to use this technique to forecast demand or find trends therein. Netto and Brei (2017) have argued that marketing research should: "combine different sources of data, such as free public data, firm property data, commercially available market research, big data, and primary data (e.g., surveys and experiments)." This article uses free public data to analyse the variations in the ownership of a white good – air conditioner in this case – across different states in India and its relationship with certain macro-economic indicators. The indicators chosen are total number of households (TH), Gross State Domestic Products (GSDP), Per Capita Income (PCI) and GSDP Growth Rate (GR).

Artificial Neural Networks: Artificial neural networks (ANNs) are biological nervous systems-inspired computational networks. In fact, an ANN is a first-order mathematical approximation to the human nervous system. It is a computational model with several processing elements. These elements take inputs and give outputs based on predefined activation functions. ANNs are used to solve various nonlinear problems. For a detailed discussion, please refer to Mishra and Datta-Gupta (2018).

Macro-economic Factors and Durable Goods Consumption: Durable goods consumption has been found to lead GDP over the business cycle. It is also an indicator of the future path the GDP may take. If durable goods consumption is found to be above its trend, then the GDP of the next quarter can also be expected to be above the trend (Carroll 2012). Similarly, increase in number of households has been found to correspond to the registration of new cars (Atkinson 1950). Growth rate of Gross State Domestic Product (GSDP) is an important parameter in the measurement of a state's economic performance and also contributes to the measurement of the performance of the country as a whole. It is defined as "a measure, in monetary terms, of the volume of all goods and services produced within the boundaries of the State during a given period of time, accounted without duplication" (data.gov.in 2015). The same source defines per capita income as: "Per capita income, also known as income per person, is the mean income of the people in an economic unit such as a country, state or district. It is calculated by taking a measure of all sources of income in the aggregate (such as GDP or Gross national income) and dividing it by the total population of country, state or district."

Indian White Goods Market: Product classification found in the textbooks generally does not further classify consumer durables. In the industry lexicon, they are further classified into two: 1) Consumer Appliances and 2) Consumer electronics. Consumer appliances are further divided into 1) White Goods, and 2) Brown Goods. However, this 'colorful' classification is not based on any clear-cut distinction among the two categories, except for the fact that historically, the white goods were made in white color, and brown goods in (dark) brown color. Though now a days these durables can be found in many different colors, the color-based category names have stuck.

Examples of white goods are washing machines, refrigerators and air conditioners. Brown goods examples are microwave ovens, cooking range, and vacuum cleaners, etc. Audio and visual systems, computers and peripherals, mobile phones, and gaming consoles, etc are put under consumer electronics. It is interesting to note that the Ministry of Statistics and Programme Implementation includes many more products, ranging from kitchenware, automobiles, gold and diamond gems and jewellery, readymade garments, footwear and even stationery items under consumer durables category in the Index of Industrial Production (IIP). However, the industry refers to only those goods as consumer durables that are generally associated with the use of electricity (Care Ratings, 2018). Despite India's climatic conditions, the penetration of domestic air conditioners is low (at about 4%) as compared to the global average of 30% (IBEF June 2019). AC penetration also lags other white goods like refrigerators (30-33%), air coolers (15-17%) and washing machines (10-11%) (HDFC Securities Nov 2019). However, there are many growth drivers which are expected to give a fillip to the sales of AC in India. Some of those factors are government focus on housing for all, rural electrification, power for all, easier access to credit, improving standard of living and changing lifestyles, higher disposable incomes, energy-efficient AC technology, and inverter-powered AC technology, etc.

OBJECTIVE OF THE STUDY

To analyse if the variations in the ownership of a white good, in this case AC, across states in India show any relationship with the variations across the states in terms of certain macro-economic indicators.

MATERIALS AND METHODS

Software used: The analysis of data for this article was done using the Pipeline Pilot module of Biovia, a proprietary software of Dassault Systemes of France. The software provides different built-in components to develop a machine learning model and use the same for prediction. The module uses data pipelining engine to execute data processing procedures which are developed within the Pipeline Pilot graphical authoring environment. The module thus helps in the development, standardization, and automation of scientific data management, analysis and reporting (Dassault Systèmes 2015).

Collection of data: Secondary data was collected from a 2018 report on room air conditioner market in India by Motilal Oswal Financial Services Ltd. The state wise macro-economic data was collected from the website of The Economic and Statistical Organization of Punjab. The reasons these reports were selected were their easy availability on the Internet and also availability of the data related to the study objective. Year 2011 was selected as the year of study to examine the relationships between the variations because this year was the last census year and data was available in the reports cited above. Those states whose data could not be found in both the reports were not considered for analysis. The states whose data was taken up are: Andhra Pradesh, Bihar, Chhattisgarh, Goa, Gujarat, Haryana, Jharkhand, Karnataka, Kerala, Madhya Pradesh, Maharashtra, Odisha, Punjab, Rajasthan, Tamil Nadu, Telangana, Uttar Pradesh, and West Bengal, and the UTs of Delhi and Chandigarh. The data were normalized within the range of minimum and maximum for each parameter such that all the values lie between 0 and 1. The data were randomized and fed into a neural network model.

Development of deep learning neural network model: The normalized dataset was read using "Delimited Text Reader" component of pipeline pilot. The component was connected to the "Learn R Deep Neural Net Model" component. The output of the model was displayed using "HTML Table Viewer" component (Fig 2). The parameters for the "Learn R Deep Neural Net Model" component were set as shown in Figure 3. The setting for which the experimental output parameter and the predicted parameter were close to a 45^0 line were considered for the final model.

RESULTS AND DISCUSSION

GSDP Growth Rate and Predicted AC Sales: The chart in Fig 5 shows that higher the achievement of growth rate in GSDP of a state in the select list of states, higher is the ownership of ACs. But as the growth rate approaches the highest in the group, the number of AC ownership is slowing down and reaching a peak. This trend implies that the states with lesser achievement of GSDP growth rate present higher AC sales opportunities than the states with higher achievement of GSDP growth rate. So, the AC manufacturers should focus more on such states to build their markets.

GSDP and Predicted AC Sales: This chart (Fig 6) is in line with the previous one on growth rate of GSDP with the exception that the predicted AC sales is peaking up in the states whose GSDP is just above the median value. This implies that states with higher GSDP are mature markets for ACs. However, it is to be noted that this chart, as the other three, shows trend between AC ownership and GSDP of states keeping the other three macro-economic

factors under study constant. In other words, keeping the number of households, per capita income and higher achievement of GSDP growth rate constant, the AC ownership is found to be increasing with higher GSDP states till the median value, after which it is slowing and eventually coming down. It can be posited that states with higher GSDP are matured markets, and that beyond a certain level of GSDP, AC ownership is coming down as the indicator total number of household has been kept constant.

Per Capita Income and Predicted AC Sales: This chart (Fig 7) shows that states with higher per capita income (PCI) are having higher AC ownership and that with increase in PCI, the predicted AC sales will increase. This finding is in the expected line. So, AC manufacturers can pay extra attention to states with growing per capita income and should keep the impact of this indicator in mind while using the judgemental methods of demand estimation of their products state wise.

Total number of Households and Predicted AC Sales: Total households (TH) indicator (Fig 8) is found to be having a positive trend for predicted AC sales (PAC). In other words, increase in number of households would increase the AC ownership even when the other three indicators have been kept constant. This can be explained by the facts that factors like increased electrification, availability of energy-efficient star-rated ACs, availability of inverter-operated ACs, better invertors because of better battery technology and hotter climates are expected to spur the growth in the AC ownership.

CONCLUSION

Publicly available data could be useful for estimation of future demand. There are a number of judgemental and statistical methods for demand and sales forecasting. Suitable methods from both the categories could be used and integrated to improve the accuracy of the forecast. Macro-economic indicators are important in predicting future sales. Machine Learning using the Artificial Neural Network is an useful method of predicting sales using macro-economic parameters. This article has used four such indicators, viz, Number of Households, Gross State Domestic Product, Growth rate in GSDP, and Per Capita Income for eighteen states and two union territories in India to find trends in the AC sales. In the states with higher growth rate (GR) and GSDP, AC ownerships found to be saturating as compared to those with relatively lower values for these two indicators. The other two macro-economic indicators, i.e., total number of households (TH) and per capita income (PCI) were found to be steadily proportional to the AC ownerships.

Suggestion for Future Research: Further research can be done in case of other white and brown goods to find the impact of the macro-economic indicators used in this article or any other set or combinations of such indicators. Another useful research could be a model that could use the ownership data of one type of consumer durables by households, in addition to suitable other data, as input and predict sales of some other durable.

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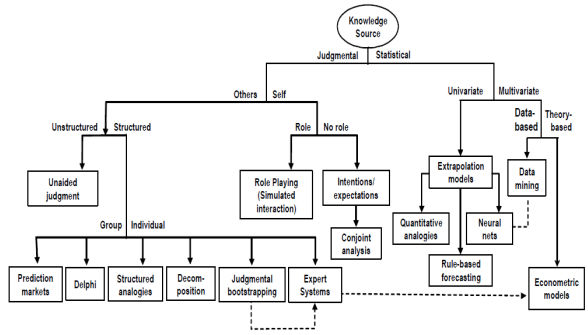


Figure 1. Characteristics of forecasting methods and their interrelationships. Source: Armstrong (2008), p2.

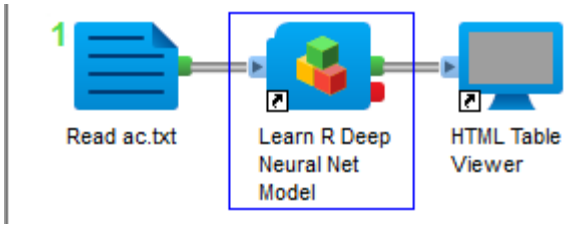
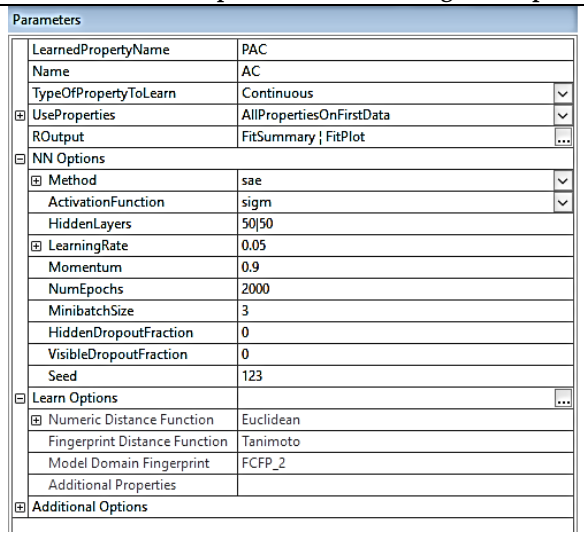


Figure 2. Artificial Neural Network Model



Parameters	
LearnedPropertyName	PAC
Name	AC
TypeOfPropertyToLearn	Continuous
⊞ UseProperties	AllPropertiesOnFirstData
ROutput	FitSummary ¦ FitPlot
⊟ NN Options	
⊞ Method	sae
ActivationFunction	sigm
HiddenLayers	50|50
⊞ LearningRate	0.05
Momentum	0.9
NumEpochs	2000
MinibatchSize	3
HiddenDropoutFraction	0
VisibleDropoutFraction	0
Seed	123
⊟ Learn Options	
⊞ Numeric Distance Function	Euclidean
Fingerprint Distance Function	Tanimoto
Model Domain Fingerprint	FCFP_2
Additional Properties	
⊞ Additional Options	

Figure 3. Parameters for the "Learn R Deep Neural Net Model" component

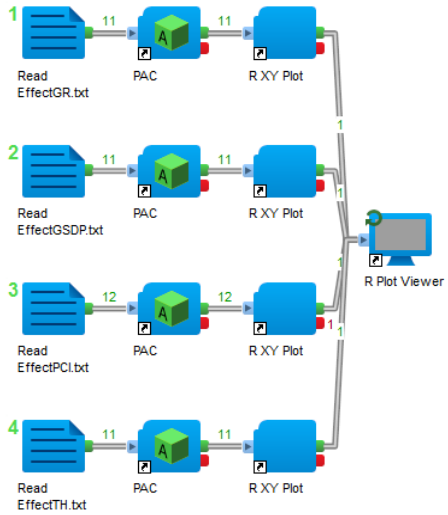


Figure 4. Use of trained model for prediction

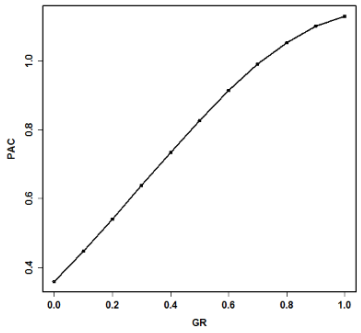


Figure 5. Effect of GSDP Growth Rate on Predicted AC Sales

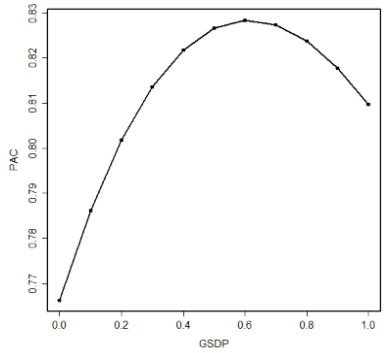


Figure 6. Effect of GSDP on Predicted AC Sales

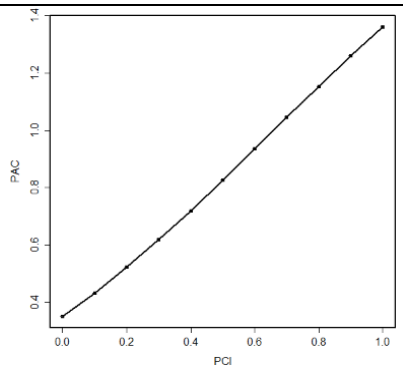


Figure 7. Effect of Per Capita Income on Predicted AC Sales

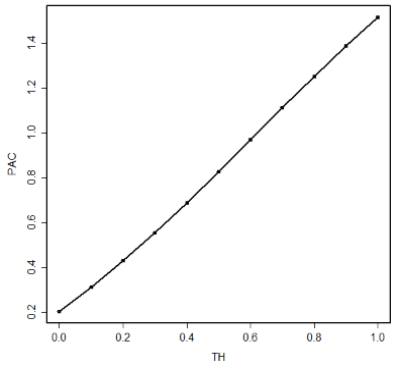


Figure 8. Effect of Total number of Households on Predicted AC Sales

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RESEARCH ARTICLE

Trends in Household Savings and Investments during FY 1998-FY2015- An Analysis

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ABSTRACT

Savings, investments and economic growth are interrelated and interdependent. A number of economic models and large number of studies have attempted to explain and establish these interrelationships and interdependencies with divergent results. The direction of causality also has been shown to be different by different models and studies. In India, the household sector contributes the most to the gross domestic savings though it has been declining in the last few years. The composition of household savings and investments are skewed towards physical assets and currency holding as well as deposits respectively. This study takes data on composition of the Indian household savings and investments for a period of eighteen years before the 2016 demonetization year, i.e., FY 1998-2015 to explore the interrelations among the various components of household saving and investments.

Keywords: Household sector, Household savings, Household investments, Trends in Household savings in India, Trends in Household investments in India, Financial years 1998-2015.

INTRODUCTION

Savings, investments and economic growth are interrelated and interdependent (Anwar and Sampath, 1999, Piotr, 2011, The World Bank, 2013). A number of economic models and large number of studies have attempted to explain and establish these interrelationships and interdependencies with divergent results. The direction of causality also has been shown to be different by different models and studies.

In India, the gross domestic saving, as a percentage of gross domestic product, has consistently increased post-Independence. Private savings have far exceeded the public savings, which in fact has declined from early 1980s.

Within private savings, the household savings has been contributing the maximum to the domestic savings (Roy Choudhury and Bagchi, 1990, encyclopedia.com 2000).

In India, the household sector contributes the most to the gross domestic savings though it has been declining in the last few years. The composition of household savings and investments are skewed towards physical assets and currency holding as well as deposits respectively. This study takes data on composition of the Indian household savings and investments for a period of eighteen years before the 2016 demonetization year, i.e., FY 1998-2015 to explore the interrelations among the various components of household saving and investments.

Typology: This section presents the definitions of the pertinent terms adopted by official bodies such as Government agencies like the central banks and the keepers of economics and other statistics.

Savings and Savings Rate: Savings is simply total income less total expenditure. Savings rate refers to the amount a person, household or an organization puts in the savings account or a similar avenue as a percentage of the total disposable income of that person, household or organization.

Gross Domestic Savings: Domestic savings have three components – Household sector savings, private corporate sector savings and public sector savings.

Household sector: European System of National and Regional Accounts (ESA 2010) defines Household sector as: "…consists of individuals or groups of individuals as consumers and as entrepreneurs producing market goods and non-financial and financial services (market producers) provided that the production of goods and services is not by separate entities treated as quasi corporations. It also includes individuals or groups of individuals as producers of goods and nonfinancial services for exclusively own final use." Ministry of Statistics and Programme Implementation MOSPI (2007), India, includes in the household sector all "individuals, all non-government, non-corporate enterprises like sole proprietorships and partnerships owned and/or controlled by individuals and non-profit institutions which furnish educational, health, cultural, recreational and other social and community services to households."

Household sector has been termed as the net financial surplus sector in the economy (Prakash et al March 2018). Among the three sectors mentioned above, household sector is the most heterogeneous sector. It includes not only resident household, but also non-profit private entities serving the households and quasi-corporate sector. However, when base year of national accounts was changed to 2011-12 from 2004-05, the definition of Household sector was also changed slightly. Now, all the quasi-corporates, who prepare their accounts in the same way as the private registered and listed corporates, have been placed under the private corporate sector category. Unregistered MSMEs (micro, small and medium enterprises) are also placed under the household sector (Suneja, 2018).

Household Sector Savings: It is the savings out of the disposable income of households. It has two components – saving in financial assets and saving in physical assets. Saving in financial assets is gross financial assets less financial liabilities. Gross financial assets include savings in various avenues such as currency (cash holdings), bank and non-bank deposits (e.g., NBFC deposits), different types of provident funds, pension funds, life insurance, stocks, debentures, mutual funds, claims on government (post office and small savings schemes), and net trade debt. Financial liabilities include loan and advances from bank and non-bank sources, housing finance companies, cooperative non-credit societies, and government sources. Physical assets include house, real estate, gold and silver.

Household Investment Rate: It is defined as gross investment divided by gross disposable income of the household sector in national accounts. Purchase of consumer durables including passenger cars, are not part of household investment.Contribution of the public sector to the gross investments used to be highest till the economic

liberalizations and privatizations gained momentum. Though household savings are the highest among the three sectors, household investments have remained in-between the other two. Out of the three sectors, the private sector is considered the most efficient investor in the economy.

Net claims on government: Ministry of Statistics and Programme Implementation, MOSPI (2007) defines this component as: "…investment in government securities, small savings, bearer bonds, capital investment bonds, national rural development bonds, national deposit scheme, compulsory deposits and other such schemes brought out by the Government from time to time, less household's net borrowing from the Government."

Trade Debt: Ministry of Statistics and Program Implementation, MOSPI (2007), defines the trade debt (net) as "the change in trade due in respect of sundry creditors minus change in loans and advances to sundry debtors.

Importance of Household Savings for a Country's Economy: Household financial savings are the most important source of investment for any economy. Out of the three sectors, the household savings historically has the largest share in gross domestic savings (Krishnamurty and Saibaba 1981). Traditionally, this sector also has been a financial surplus sector. In an ideal economic situation, household is the net lender to the economy, with public sector a net minor borrower and private sector a major net borrower.

Recent Trends in Household Savings in India: Till the FY 2012, India's aggregate savings rate was comparable to the emerging economies in Asia like Thailand and Indonesia. It was even much higher than that in the developed economies like the USA and the UK. However, from the year 2011-12, 2016-17 and beyond, the household savings rate has been on steeply downward trend - 23.64 per cent of GDP in 2011-12 to 16.26 per cent in 2016-17 (Rangarajan, 2018). Savings in both physical assets as well as financial assets are part of this decline. Post-demonetization, the savings pattern has swung from physical assets to financial assets, with bank deposits continue to corner the lions share (but declining - from 56% in FY12 to 41% in FY16) and mutual funds gaining currency (ICICI Securities 2016). Interestingly, 2018 RBI data shows that the cash holdings are at the highest level since 2011, proving the apprehension that people have reverted to their old having of saving in cash (Business Today 2018).

REVIEW OF LITERATURE

The relationship between savings, investment and growth have been examined by different economic models like the neo-classical growth models of Ramsey (1928), Solow (1956), Swan (1956) Cass (1965), and Koopmans (1965), and the AK models of Harrod (1939), Domar (1946), Frankel (1962) and Romer (1986).

There have been divergent views on what drives economic growth among the economists, policy makers and researchers– savings, investments or consumption. For example, Lewsi (1955) has propounded that an increase in savings accelerates economic growth. Solow (1956) model has argued that there is a virtuous cycle between income, saving and investments – income raises saving, which in turn raises investments. The early Harrod-Domar models, on the other hand have advocated the prime role of investments for the economic growth **(**Jangili 2011)**.** Jappelli and Pagano (1994) have argued that higher saving leads to higher investment which in turn leads to higher GDP growth, but in the short-run. While all these models have assumed that savings is the cause and investments and economic growth as the effects, Carroll and Weil (1994) have hypothesized to the contrary that it is economic growth which is the cause of savings and not the other way round.

As far as consumption is concerned, it may be financed by savings or higher disposable income. On the current debates on the economic growth in India, some analysts have advocated consumption-led growth rather than domestic investment-driven growth, particularly, investments by the private sector (Gupta 2016).

Researchers in the Indian context have found support for the above divergent views on the interrelationships or interdependencies among savings, investments and economic growth (Sinha, 1996, Mühleisen, 1997, Sinha and Sinha, 2008, Verma, 2007, Verma, 2009, Samantaraya and Patra 2014). Singh (2010) in his study on the long-run effects of domestic saving on income found bidirectional causality between saving and growth. Jangili (2011), testing for Granger causality between saving, nominal investment and nominal GDP in India at aggregate and sectoral levels, found evidence of the direction of causality from saving and investment, both individually as well as collectively, to economic growth, but not the other way round. However, his study found the reciprocal causality between saving and investment in case of the household sector.

Out of the different savings options, Indian households have found to prefer physical assets like land, buildings, gold, machinery and livestock which are not as liquid as the financial savings (Patrick 2015). Among the financial savings, bank deposits have taken precedence over the other forms of savings like life insurance, shares and debentures, etc. As household savings has the largest share (almost 70%) in the gross domestic savings in India, there is a need to study the trends in it and its components and their interrelationship/ interdependencies with household investments. This article examines these trends and interrelationships between household savings, and its components, and household investments and its major components for the period between FY 1998 and FY 2015. The period covers eighteen financial years before the 2016 demonetization in India.

OBJECTIVES OF THE STUDY

The study analyzes the interrelationships/Interdependencies among the components of Total Household Savings, i.e., Gross Financial Savings, Physical Savings and Financial Liabilities. It also analyses the interrelationships/Interdependencies among the components of Total Household Investments. The same between the components of Total Household Savings and Total Household Investments has also been analyzed. The study period spans over eighteen years before the year of recent demonetization in India, i.e., FY 2016.

METHODOLOGY

Data for analysis were obtained for this exploratory study from a report by Motilal Oswal Securities Ltd (Gupta, 2016) which in turn had used data from Central Statistical Organization, Reserve Bank of India and its own reports. The data pertains to Total Household Savings as a percentage of GDP and Total Household Investments as a percentage of Gross Financial Savings from FY 1998 to FY 2015. Further granularity of both the major indicators were obtained from the same report in the form of Gross Financial Savings, Physical Savings and Financial Liability for Total Household Savings, and Currency, Deposits, (explanation of currency and deposits) Life Insurance, PF & Pension, Shares & Debentures, Claims on Government and Others (Units of UTI and trade debt (net)) for Total Household Investments.

The correlations between these indicators were studied based on the r values and p values obtained from the correlation matrix (Table 2 and Table 3) using MATLAB. r value provides not only the dependency, but also the direction of dependency, such as a value close to zero indicates no dependence. Value close to +1 or -1 indicates dependence. A +ve value shows an increase in values when the same of any of the other indicators also increases. A – ve value indicates the opposite trend. In case of p value, it is less than 0.05, it is usually considered as statistically significant. Thus this study used the r and p values to present the trends in the effect of the household savings and investment related indicators on one another.

RESULTS AND DISCUSSION

A glance at Table 1 reveals that in certain years, financial savings had exceeded the traditional physical savings. The years were 1998, 1999, 2006, and 2008. From 2011 to the end of the study period, people had significantly preferred

the physical savings routs. However, the savings in financial assets as a percentage of GDP had steadily increased till 2008, the year in which the market had crashed significantly. Currency holdings had been steady except for the period 2005-2008 when it had come down to single digit percentage point. Deposits had constituted the major share of financial savings and had steadily increased from 2006. Share of life insurance in the gross financial savings had steadily increased without any exception in any FY. On the contrary, Provident Fund and Pensions share had steadily come down from 2002 to 2014 and had gone up marginally the next FY. Share of savings in market instruments had also come down steadily over the years with a small spike in 2008. Claims on governments had upward trend between 2000 to 2006 after which it had declined significantly year after year. The last column had also steadily declined. The data is consistent with the opinion that India had been largely a cash economy. Households largely put safety of savings ahead of returns.

Claims on government (government securities, small savings, bearer bonds, etc) has significant contribution to gross household savings. Physical savings positively correlated with life insurance. Same relationships have been found between Currency and Others, PF & Pension and Shares & Debentures, PF & Pension and claims on government, and finally, PF & Pension and Others. Weak but significant relationship is found between Gross financial savings and Shares & Debentures. Negative significant correlations are there between Physical savings and PF & Pension, Physical savings and Shares & Debentures, Physical savings and Others, Financial liabilities and Currency, Financial liabilities and Others, Deposits and Shares & Debentures, Life Insurance and claims on government, and Life Insurance and Others.

CONCLUSION

An analysis of the of the composition of the Household Gross Financial Savings and Household Investments during the period FY 1998 – FY 2015 in India shows results consistent with earlier studies and reports by the central bank and other analysts. In the pre-demonetization years, India had been largely a cash economy and continues to remain so. Physical assets (mainly house and real estate) and deposits rule the roost on the savings and investment charts. Currency holding had been steady in both pre and post-demonetization years. Share of Life insurance in the total household investments had gone up with physical savings. PF & Pension and Shares & Debentures have moved together. A few years down the line, a comparative study of the compositions of household savings and investments in the pre and post-demonetization years would help the Banking, Financial Services and Insurance sector to strategize their marketing strategies to sway the Indian public more towards investments in market-related products.

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Table 1: Composition of Household Savings and Investments

	% of GDP			% of GROSS FINANCIAL SAVINGS						
FY	GROSS FINANCIAL SAVINGS	PHYSICAL SAVINGS	FINANCIAL LIABILITY	CURRENCY	DEPOSITS	LIFE INSURANCE	PF & PENSION	SHARES & DEBENTURES	CLAIMS ON GOVT	OTHERS*
98	9.3	8.7	1.6	11.2	43.7	9.4	17.9	6	9.1	2.8
99	10	9.5	1.5	11.1	43.5	9.6	18.5	5.5	9.7	2.1
00	10.2	11.5	1.8	10.8	42.5	10	19.1	5.7	10.1	1.8
01	9.9	11.4	1.5	10.2	42.1	10.5	19.3	5.6	10.8	1.5
02	10.5	12.6	2.2	10.2	41.8	11	18.8	5.3	11.7	1.3
03	10	12.3	2.4	10.0	41.8	11.6	18.2	4.9	12.4	1
04	11	12.1	2.5	10.1	41.6	11.8	17.5	4.6	13.8	0.6
05	10.1	13.4	3.7	9.9	41.3	12.3	16.8	4.2	15.1	0.4
06	11.9	11.7	5.0	9.7	41.9	12.6	15.9	4.4	15.1	0.3
07	11.3	11.9	6.6	9.6	44.3	13.0	14.9	4.8	13	0.4
08	11.6	10.8	3.8	9.7	45.2	14.2	14.1	5.5	10.7	0.6
09	10.1	13.5	2.9	10.1	46.9	15.0	13.6	4.8	9	0.6
10	12.0	13.2	3.1	10.0	46.2	16.6	13.6	4.8	8.4	0.5
11	9.9	13.2	3.6	10.4	46.9	16.9	13.5	4.2	7.6	0.5
12	7.4	15.9	3.3	10.5	47.9	17.3	13.2	3.9	6.6	0.5
13	7.4	14.7	3.3	10.5	48.8	17.3	13	4.0	5.9	0.5
14	7.7	13.0	2.7	10.2	50.3	17.2	12.8	3.8	5.3	0.5
15	7.7	11.0	2.3	10.2	50.2	17.4	13.1	3.9	4.8	0.5

* Units of UTI and trade debt (net) Source: Gupta (2016)

Table 2: The r Values

r value	GROSS FINANCIAL SAVINGS	PHYSICAL SAVINGS	FINANCIAL LIABILITY	CURRENCY	DEPOSITS	LIFE INSURANCE	PF & PENSION	SHARES & DEBENTURES	CLAIMS ON GOVT	OTHERS*
GROSS FINANCIAL SAVINGS	1	-0.3234	0.3268	-0.4547	-0.6524	-0.4393	0.3397	0.4761	0.7389	-0.0268
PS PHYSICAL SAVINGS	-0.3234	1	0.3002	-0.2978	0.3605	0.6578	-0.5251	-0.6982	-0.2159	-0.6806
FINANCIAL LIABILITY	0.3268	0.3002	1	-0.6889	0.0632	0.3224	-0.4588	-0.3895	0.3156	-0.6671
CURRENCY	-0.4547	-0.2978	-0.6889	1	0.0816	-0.2760	0.2940	0.3372	-0.4315	0.7838
DEPOSITS	-0.6524	0.3605	0.0632	0.0816	1	0.8675	-0.8658	-0.5939	-0.8975	-0.3658
LIFE INSURANCE	-0.4393	0.6578	0.3224	-0.2760	0.8675	1	-0.9505	-0.8052	-0.6555	-0.7303

PF & PENSION	0.3397	-0.5251	-0.4588	0.2940	-0.8658	-0.9505	1	0.7225	0.5929	0.6948
SHARES & DEBENTURES	0.4761	-0.6982	-0.3895	0.3372	-0.5939	-0.8052	0.7225	1	0.3246	0.7984
CLAIMS ON GOVT	0.7389	-0.2159	0.3156	-0.4315	-0.8975	-0.6555	0.5929	0.3246	1	-0.0044
OTHERS*	-0.0268	-0.6806	-0.6671	0.7838	-0.3658	-0.7303	0.6948	0.7984	-0.0044	1

Table 3: The p Values

p value	**GROSS FINANCIAL SAVINGS**	**PHYSICAL SAVINGS**	**FINANCIAL LIABILITY**	**CURRENCY**	**DEPOSITS**	**LIFE INSURANCE**	**PF & PENSION**	**SHARES & DEBENTURES**	**CLAIMS ON GOVT**	**OTHERS***
GROSS FINANCIAL SAVINGS	1.0000	0.1905	0.1857	0.0580	0.0033	0.0682	0.1678	0.0458	0.0005	0.9160
PHYSICAL SAVINGS	0.1905	1.0000	0.2261	0.2301	0.1417	0.0030	0.0252	0.0013	0.3895	0.0019
FINANCIAL LIABILITY	0.1857	0.2261	1.0000	0.0016	0.8033	0.1919	0.0555	0.1102	0.2020	0.0025
CURRENCY	0.0580	0.2301	0.0016	1.0000	0.7476	0.2676	0.2363	0.1711	0.0738	0.0001
DEPOSITS	0.0033	0.1417	0.8033	0.7476	1.0000	0.0000	0.0000	0.0094	0.0000	0.1355
LIFE INSURANCE	0.0682	0.0030	0.1919	0.2676	0.0000	1.0000	0.0000	0.0001	0.0031	0.0006
PF & PENSION	0.1678	0.0252	0.0555	0.2363	0.0000	0.0000	1.0000	0.0007	0.0095	0.0014
SHARES & DEBENTURES	0.0458	0.0013	0.1102	0.1711	0.0094	0.0001	0.0007	1.0000	0.1888	0.0001
CLAIMS ON GOVT	0.0005	0.3895	0.2020	0.0738	0.0000	0.0031	0.0095	0.1888	1.0000	0.9860
OTHERS*	0.9160	0.0019	0.0025	0.0001	0.1355	0.0006	0.0014	0.0001	0.9860	1.0000

From the above two tables, following observations could be drawn:

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RESEARCH ARTICLE

Effectiveness of Dyadic Communication of Farm Family Heads with Their Daughters

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ABSTRACT

Dyadic communication is a deep interpersonal communication between two dyads. The two dyads interact with each other very frequently for a common purpose. There are communications between various dyads such as husband-wife, father-son, father-daughter, teacher-student, and supervisor-supervisee. At present, farmers are facing a number of stresses as they work in isolation and have to put in long hours with little time for rest and recreation. This leads to depression. Generally, farmers' families are dependent on the family household heads for their sustenance. If proper relationships exist between the various dyads in the family, in times of uncertainty a wife, son or daughter can be of immense help to a farmer in surmounting the various difficulties and stresses faced during farming.

INTRODUCTION

Communication is the process of exchange of ideas, feelings, thoughts, and messages with others [1]. Dyadic communication is of central importance to interpersonal relationships. Dyads exit in families, work groups, neighbours, or students in a class. A large group breaks down into a series of dyads. Dyads are formed for achieving a mutually desired benefit or goal. Two people may form a group in an organization for improving the work morale. Husband and wife, a dyadic group, if faced with marital difficulties may form a coalition with one their children. Due to the relationship, a dyadic consciousness emerges and they see that they work as a pair, a team, or a couple [2]. A dyadic communication is an interpersonal communication and it is a transaction that takes place between two

individuals [3]. As the elements in the communication process determine the quality of communication, a problem in any of the statements can reduce communication effectiveness [4]. Selection of the particular medium for transmitting the message can be critical, because there are many choices. Information must be encoded into a message that can be understood as intended by the sender. There are many choices for transmitting the messages. Due to differences in language, education, and culture, semantic barriers come into play. Semantic barriers come from differences in language, education, and culture. Obviously, there is a problem if the sender is speaking in a language the receiver does not understand.

Objectives

(1) To study the dyadic communication pattern between farm family head and daughter for taking farming decisions
(2) To find out the distance maintained while communicating in different dyadic situations among the dyad, farm family head and daughter.

MATERIALS AND METHODS

In Ganjam district in Odisha the blocks Digapahandi and Chikiti were purposively selected for the study. Two villages Gadagovindapur and B-Nuapada were randomly selected under these two blocks. From each village fifty farmers were taken from the two blocks. For the study Purposive as well as simple random techniques were adopted. While selecting districts and blocks purposive sampling technique was adopted. Simple random sampling technique was adopted for selection of villages and respondents. The total number of farm respondents was one hundred under the study. Dyadic communications among the farm family members with respect to the farming activities were the dependent variable of the study.

ANALYSIS

Table 1 represents the communication between the family heads and their daughters. The variable education of the respondent, family education status, and family size were significantly associated with the dyadic communication with daughters with respect to farming operations. The education of the respondent and the family education status were negatively and significantly associated with the dyadic communication between father and daughter. The possible explanation is that due to the differences of education status, the mental distance between the elements of the dyad increased to a considerable extent. Effectiveness of communication in the dyad regarding farming activities was hampered due to the difference in educational status. Family education status of the respondent had also negatively significant association with the dyadic communication between a family head and his daughter. Due to the increased educational level of both individuals the information endowment regarding farming operations would be more which ultimately influences to create an antagonistic effect instead of a synergistic effect and chances of conflict may arise regarding farming operations.

Family size showed a positive and significant relationship with dyadic communication between family heads and their daughters. With the increase in number of family members, the dyadic communication between the family heads and their daughters increased. The cumulative effect of interaction between the family heads and their daughters increased the dyadic communication status of the families. It was clear that cumulative interaction offered higher communication efficiency than individual interaction. Table 2 shows that in case of the dyad family head-daughter the multiple regression analysis showed that the variable family size was positively and significantly effective in delineating the variable dyadic communication and the contribution of the variable family size is 57.40% in delineating the dyadic communication between family heads and daughters.

CONCLUSION

Social grouping is very important for human beings. The social group has a role in maintaining the relationship among the members. Various dyads exist in society. Proper dyadic communication should exist for taking firm decisions on cultivation practices and maintaining behavioral health. This can help the farmer to manage the farm in a better way and in times of distress, he can be saved.

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Table 1. Coefficient of correlation between dyadic communication and 18 causal variables

Sl No	Variables	Family Head and Daughter
1	Age(x_1)	0.1668
2	Occupation(x_2)	0.0269
3	Caste(x_3)	0.0282
4	Educational level(x_4)	-0.2189*
5	Family education status(x_5)	-0.2146*
6	Family size(x_6)	0.3506**
7	Social participation(x_7)	0.1398
8	House type(x_8)	0.0334
9	Material possession(x_9)	-0.0260
10	Land holding(x_{10})	0.1531
11	Agricultural implements(x_{11})	0.1062
12	Risk taking ability(x_{12})	0.1524
13	Cosmopoliteness(x_{13})	0.1204
14	Mass media exposure(x_{14})	0.1916
15	Fatalism(x_{15})	-0.1472
16	Dependence(x_{16})	-0.1511
17	Tolerance(x_{17})	0.0016
18	Faith(x_{18})	-0.0341

Table 2. Multiple regression analysis of dyadic communication pattern and 18 causal variables

Sl No	Variables	Standardized regression coefficient (β)	β×R	Multiple regression coefficient	SE of 'b'	t value of 'b'
1	Age(X_1)	-0.147	-10.803	-0.190	0.197	0.967
2	Occupation(X_2)	0.095	1.112	1.750	2.214	0.190
3	Caste(X_3)	0.018	0.229	0.314	1.849	0.170
4	Educational level(X_4)	-0.164	15.813	-0.638	0.491	1.301
5	Family education status(X_5)	-0.001	0.093	-0.005	0.684	0.008
6	Family size(X_6)	0.371	57.403	1.477	0.623	2.370*
7	Social Participation(X_7)	0.079	4.870	0.503	0.787	0.639
8	House Type(X_8)	-0.075	-1.110	-1.457	2.802	0.520
9	Material Possession(X_9)	-0.154	1.765	-0.390	0.348	1.121
10	Land holding(X_{10})	-0.036	-2.406	-0.038	0.166	0.232
11	Agricultural Implements(X_{11})	0.060	2.817	0.237	0.551	0.430
12	Risk taking ability(X_{12})	0.127	8.548	3.814	3.691	1.033
13	Cosmopoliteness(X_{13})	0.038	1.993	0.411	1.440	0.285
14	Mass Media Exposure(X_{14})	0.030	2.568	0.065	0.329	0.197
15	Fatalism(X_{15})	-0.121	7.879	-0.200	0.219	0.917
16	Dependence(X_{16})	-0.118	7.845	-0.438	0.413	1.060
17	Tolerance(X_{17})	-0.016	-0.011	-0.826	0.829	0.152
18	Faith(X_{18})	-0.093	1.397	-0.577	0.789	0.732

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RESEARCH ARTICLE

Genetic Control on Root Organogenesis in Cereal Crops

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ABSTRACT

Organogenesis has provided useful systems for understanding the regulatory mechanisms of plant development.After the identification of chemical determinants in plant growth and development, several studies have been carried out on molecular mechanisms responsible for organogenesis over the years.Understanding the regulation of root development is of great importance in the field of agriculture.It is a crucial determinant for plant anchorage, the efficiency of water and nutrient uptake, and establishment of plant- microbial communities.Higher plants exhibit an amazing diversity of root architecture at a morphological level. Recent genetic studies have identified several genes responsible for root initiation in cereals (Coudert*et al*., 2010). A conserved core gene regulatory network regulates root initiation.Chen *et al*. (2012) have examined the effect of Nitric Oxide and Auxin on the induction of lateral root formation in rice (*Oryza sativa* L.), by recording the HemeOxygenase (HO) activity and the lateral root number. Heme Oxygenase gene (*OsHO)* activation has a positive effect on the lateral root system. It was concluded that Nitric oxide and Auxin increase HO activity at the molecular level and in turn increase the lateral root number in rice.

Keywords: mechanisms, *Oryza sativa,* network, activity, molecular.

INTRODUCTION

Cereal crops are the essential food crop, feeding more than half of the world's population. The increasing population and economic development have been posing a growing pressure in food production. To meet the demand for food for the increasing population, raising the yield ceiling of cereals remains a priority task for breeders. As an essential organ of the rice plant, root performs vital functions: acquisition of resources and anchorage of the plant. A plant's

roots system determines both the capacity of a sessile organism to acquire nutrients and water, as well as to provide a means to monitor the soil for a range of environmental conditions. These enable a plant to shape the root architecture by its needs and the physical constraints imposed by its environment n develop a well-adapted root system. Due to the importance of roots to ensure crop yield under suboptimal water-availability or low soil fertility. The plant's root system is a critical target trait to improve crop performance. It, therefore, is relevant to acquire further insights into root formation, root architecture and the controlling physiological and genetic factor Organogenesis is a significant path of regeneration that involves differentiation of cells or tissue into organs such as shoots and roots. Organogenesis is derived from the Greek words "Organo" & "Genesis".

Factors affecting organogenesis

Intrinsic factor

Genetic control: The presence or absence of auxin transcriptionally regulates many genes involved in general root growth and development.

Hormonal control: Endogenous auxin accumulates in the root tip where it coordinates cell divisions, cell expansion and contributes to the gravitropic response of the root

Extrinsic factor

- Environmental factor
- Gravity
- Light
- Water availability
- Nutrient gradient

Roots and its characteristics: "Roots are axial multicellular structures of sporophytes of vascular plants which usually occurs underground, have strictly apical elongation growth, and generally have gravitropic responses which range from positive gravitropism to diagravitropism, combined with negative phototropism" Raven and Edwards (2001).

Different parts of roots:

Characteristics of root

i. Descending part
ii. Negatively phototrophic
iii. Non-green
iv. Root cap /root pockets
v. Unicellular root hair
vi. No nodes
vii. Lateral roots

Incase of monocot plant root, there is no secondary growth, and vascular bundle is scattered. Incase of dicot plant root, secondary growth is present, which make an annual ring and also vascular bundle compactly packed.

Root organogenesis: The root system 's fundamental function is to mediate contact between plant and soil, and to provide water and nutrients to the plant. The root system 's architecture is determined by endogenous mechanisms which integrate constantly.Environmental signals, such as nutrient availability and moisture or salinity, and thus modulation of the primary root growth and branching. The developmental Root flexibility systems which are extremely important for the efficient use of soil and the survival of plants under less favorable conditions are largely determined by their post-embryonic branching ability. Lateral roots originate from selected pericycle cells which

acquire the attributes of founding cells and subsequently undergo a series of anticlinal divisions. The architecture of the root system largely depends on the development of individual root initiation events controlled by spatiotemporal regulation.

Importance of genetic improvement of root

Increasing productivity: The grain filling in rice is found to increase with the increase in the root activity improved at a genetic level. (Yang *et al.,*2011).Success in "super" rice breeding has been considered significant progress in rice production in China. This study aimed to test the hypothesis that an improved root system may contribute to better shoot growth and consequently to higher grain yield in "super" rice.

Enhancing tolerance to abiotic stresses: Improvement of plant roots at the genetic level help develop new varieties of crops. which can survive drought, and produce higher yields under water-scarce farming systems. (Gowda*et al.,*2011) . Genetically improving the root system help plants tackle abiotic stresses like high soil salinity. The plants developed to have root systems which have low affinity for toxic K+ ions or have a low Na+ to K+ ratio. Due to high NaCl quantity in soil, the plant roots protect the plant against the toxic effects of Na+ ions and maintains the efflux of Na+ with the influx of K+ ions into the roots. (Horie*et al*2011).

Improving the efficiency of nutrients: Developing cultivars with genetically regulated root systems which can utilize soil nutrients effectively and not rely on fertilizer application alone. (Wada *et al*1990) .

Genetic control of root organogenesis by NO_3^-. : NO, and auxin act synergically to control diverse aspects of root biology and lateral root development. Nitrate is firmly auxin-dependent, a role of NO as a coordinator of nitrate and auxinsignalling to control the overall root response. The high rate of N supply to the root system as a whole usually is associated with a reduced allocation of resources to root growth (i.e., decreased root/shoot ratios). Similar contradictory effects of NO3 on root growth were observed. It was proposed that the NO3 supply modulates lateral root (LR) development in two distinct ways through a systemic inhibitory effect that results from the accumulation of NO3 (and/or its metabolites) in the shoot. Another through a localized stimulatory effect that depends on the local concentration of NO3 at the LR tip. An analogous ''feedback–feedforward'' model for NO3 regulation.

Genes responsible for root organogenesis: Genetic and molecular mechanisms controlling root development is critical for the development of new rice ideotypes. Those are better adapted to adverse conditions and for the production of sustainably achieved rice yield potential.

Genetic control on root organogenesis by Auxin.: Root development in cereals is controlled by many extrinsic (environmental) and intrinsic signals. Plant hormones represent critical regulators of plant developmental processes, including lateral root initiation, patterning, and the emergence of the lateral root. Besides the classical phytohormones, peptide hormones such as members of the CLE-Like/GOLVEN family small molecules such as nitrite oxide, or reactive oxygen species also have regulatory effects on different aspects of root development and branching.

PIN-FORMED (PIN) and AUX1 classes of auxin efflux and influx carriers are involved in lateral root formation in cereals. PIN auxin efflux carriers, such as ETHYLENEINSENSITIVE ROOT (EIR) and AUX1 influx carriers are expressed in specific areas of the root about lateral root formation, in riceand barley respectively. The maize homologue of AUX1is also highly expressed during brace root initiation.Mutations in the rice gene crown rootless4 (crl4) and Osgnom1 exhibit no crown roots and a reduced number of lateral roots . Also, the expression of OsPIN2, OsPIN5b, and OsPIN9 is altered inOsgnom1, indicating that polar auxin transport involving OsPINauxin carriers and regulated by CRL4/OsGNOM1is required for crown root and lateral root initiation in rice. AUXIN/INDOLE-3-

ACETIC ACID (Aux/IAA) proteins are critical regulators of the nuclear auxin response pathway and modulate lateral root formation. This proteins function as auxin co-receptors with TRANSPORTINHIBITOR RESPONSE 1 (TIR1) and closely related AUXIN SIGNALLING F-BOX (AFB) proteins. Aux/IAA proteins also function as transcriptional repressors by interacting with members of the AUXIN RESPONSEFACTORS (ARF) transcription In the presence of auxin. Aux/IAA proteins are degraded via ubiquitination by the E3 ligase Skp1–Cullin–F-box protein (SCF) TIR1/AFB complex, thereby derepressing ARF activity.Mutations in Aux/IAA proteins such as OsIAA13 in rice and ROOTLESS WITH UNDETECTABLE MERISTEMS1 (RUM1) in maize that block their auxin-mediated degradation confer lateral root defects. Mutant Osiaa13 contains a single amino acid substitution in the degron sequence required for the auxin-triggered turnover of the OsIAA13 protein Osiaa13 exhibits a lateral rootless phenotype. miRNAs OsMir393a and OsMir393b, negative regulators of the messenger RNAs OsTIR1 and OsAFB2, the rice orthologues of Arabidopsis auxin co-receptors TIR1 andAFB2also appear to be involved in lateral root initiation in rice. Overexpression of 35S::Mir393 causes a less number of crown roots and a strong auxin-resistant phenotype . In the crown root and at lateral root initiation sites The GUS reporter gene is present which is controlled by theOsMir393a promoter

GUS staining accumulates transiently in the pericycle cells during the early stages of lateral root formation. Suggesting thatOsMir393a may be involved in a regulatory feedback loop of auxinsignalling during lateral root initiation. Methyl jasmonate, nitric oxide, and auxin induce lateral root initiation in rice and it is hypothesized that this occurs via the induction of HEME OXYGENASE 1 (OsHO1) expression, through a calcium- and calmodulin-dependent signal transduction pathway OsHO1 can produce carbonmonoxide, a molecule known to promote lateral root initiation in different species. HO1 genes and carbon monoxide production may constitute a key relay in the promotion of lateral root initiation by different signals and hormones in monocots.

CONCLUSION

It is of prime importance to understand the root organogenesis at a molecular level. Identifying key root developmental genes can help identify those which explain a significant portion of natural root trait variation. It will be essential to the creation of new ideotypes that are better prepared against threats to the climate. Conversely, root QTL cloning would also disclose genes important to root production networks. This form of method can be carried out in the coming years, and results analysis will contribute to a more precise understanding of the molecular mechanisms of cereal root production.To design a root system for optimization to enhance and maximize crop performance, and has the potential to bring about the second green revolution.

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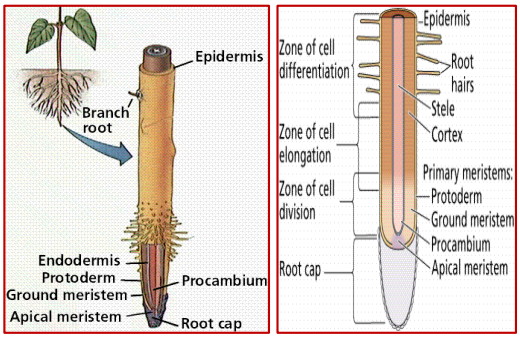
Table. 1. General organization of root:

1. Region of root cap	The tender apex of the root is protected with a multicellular cap structure called root cap.
2. Region of cell division or meristimatic region	It is the growing part of the root and is protected by the root cap.
3. Region of elongation	It just lies above the meristematic region. It increases the root.
4. Region of root hair	Surface of this area is covered with numerous root hairs
5. Region of maturation or cell differentiation	It forms the major part of the root which is covered by impermeable cells. These undergo differentiation to form tissue-like cortex, endodermis, xylem, phloem etc.

Table. 2. Genes responsible for root organogenesis

Phenotype	Gene	Reference
Radicle initiation	*RAL1,RAL2,RAL3*	**Scarpella*et al.* (2003); Hong *et al.* (1995)**
Crown root formation	*OsCAND1 , CRL1(ARL1) CRL2,CRL3 CRL4(OsGNOM1) CRL5 , WOX11*	**Wang *et al.* (2011), Woo *et al.* (2007) Zhao *et al.* (2009)**
Root elongation	*OsDGL1 , OsRR1 ,OsRR2 , OsSPR1 ,qRL6.1 qRL7 OsPIN1*	**Qin *et al.* (2013) , Kitomi*et al.* (2011) Jia*et al.* (2011), Obara*et al.* (2010) , Wang *et al.* (2013a)**
Root angle	*DRO1*	**Uga*et al.* (2013)**
Root thickness	*DES*	**Wan *et al.* (1996**
Lateral root development	*OsIAA11, OsIAA13 OsIAA23) LRT1, LRT2 , OsWOX3A(NAL2)*	**Nakamura *et al.* (2006) Zhu *et al.* (2011) Kitomi*et al.* (2012) Ni *et al.* (2011), Cho *et al.* (2013**
Root hair development	*OsAPY(RTH1) OsCSLD1 OsEXPB5,RH2, OsSRH1, OsSRH3*	**Yuo*et al.* (2009), Won *et al.* (2010) Yu *et al.* (2011)**



Root organization in dicot and monocot plants

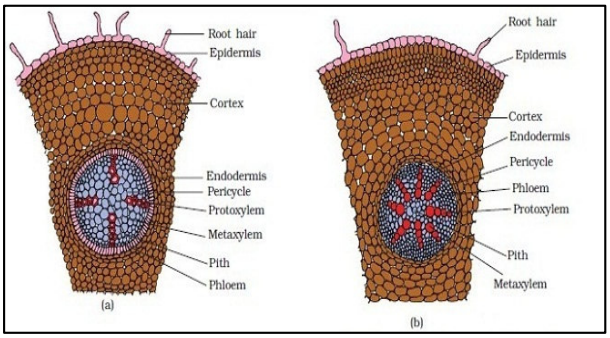


Figure.2. T.S. (a) Dicot root (Primary): (b) Monocot root

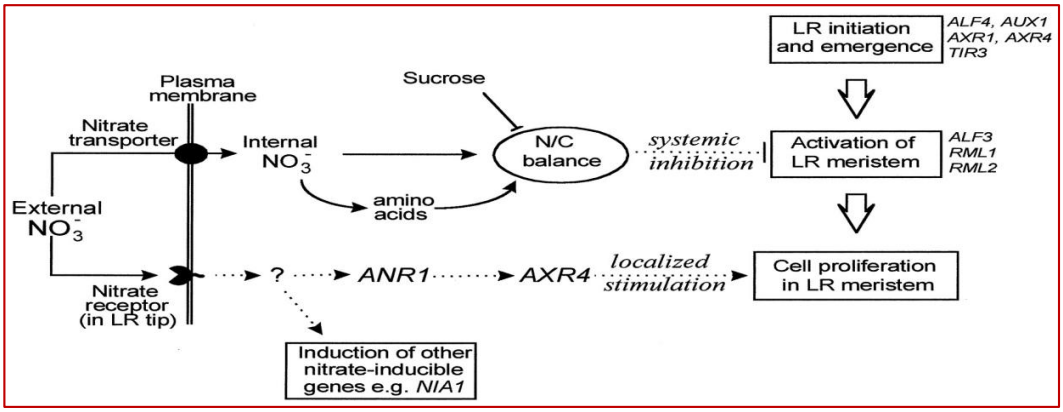


Figure.3.Genetic control of root organogenesis by NO_3^-.

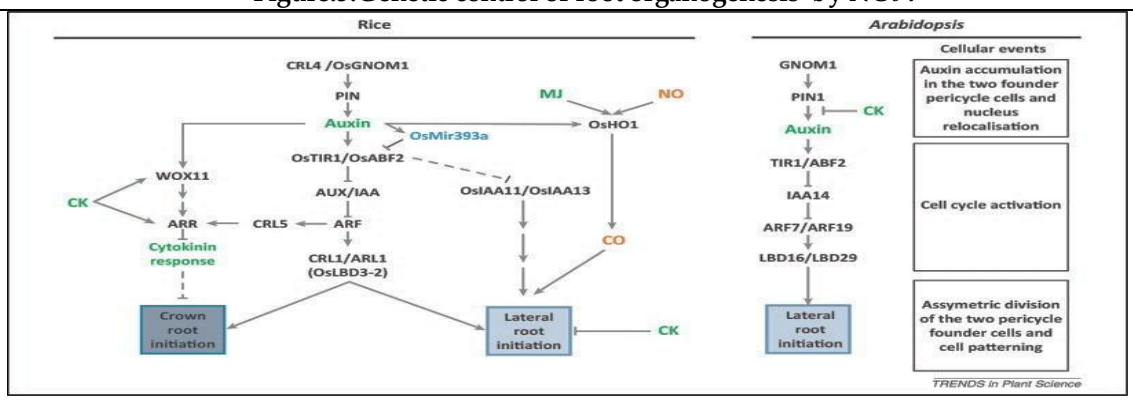


Figure.4.Genetic control on root organogenesis by Auxin.

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RESEARCH ARTICLE

New Dimensions of RNA Based Technologies in Plant Functional Genomics

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ABSTRACT

Genome sequencing not only expanded our knowledge of many plant species' blueprints but also uncovered the complexities of coding and non-coding genes. It is important to understand the basic methodolgies, design and the detail of essential RNA-based advanced technologies like a miRNA, atasiRNA, MicroRNA sponge Target mimicry,STTM,and gRNA / Cas9 for their use in plant genetic functional studies and their potential for genetic improvement of crops we addressed in this review article. The study provides perspectives on how to improve genome technologies based on the RNA and their Practical implementations in unravelling the coding and non-coding genes and their network

INTRODUCTION

Genome sequencing fostered functional genomics. The whole-genome sequences of many plant species is now available, and next tasks will be the functional verification of a large number of genes to accelerate the study of plant biology and the improvement of crop genes.Functional characterization is mainly achieved by the creation of various gain- or loss-of-function mutants in plants. Traditional gain of gene function in plants is achieved through the expression of target genes driven by strong promoters such as cauliflower mosaic virus (CaMV) 35S and CaMV 35S enhancers. Loss of gene function is commonly induced by ethane methyl sulfonate (EMS) mutagenesis or by T-DNA/transposon insertion, which leads to mutated/truncated proteins with attenuated or null functions. All these technologies target genes in a random manner without any specificity.

More recent technologies are aimed at specific gene targeting to induce loss-of-function. Loss of function can be achieved by targeting either the DNA or RNA of a specific gene for alteration or silencing. To target a specific DNA (gene) in the genome, technologies such as zinc-finger nucleases (ZFNs), transcription activator-like effector

nucleases (TALENs), meganucleases. ZFNs, TALENs, and meganucleases require complicated protein engineering before altering genes of interest. Targeting the RNA of a given gene for silencing involves the use of RNA interference (RNAi), a great discovery in silencing genes post-transcriptionally. RNA-based technologies are an essential toolbox for functional genomics in plants. Small RNA-based gene silencing is widely used as a popular means to study gene function because it can lead to gene silencing at either the transcriptional or post-transcriptional levels (target RNA cleavage or translational repression).

Understanding different types of RNAs:

Based on RNAs involved in protein synthesis, they are categorized as::
Messenger RNA (mRNA): Convey the genetic information from DNA to the ribosome.Ribosomal **RNA (rRNA):** Essential for protein synthesis.

- Transfer RNA (tRNA): Helps to decode mRNA into protein.
- RNAs involved in post-transcriptional modification:
- Small nuclear RNA (snRNA): this RNA involved in splicing mechanism.
- Small nucleolar RNA (Sno RNA): Helps to chemical modification of other RNA.
- Guide RNA (gRNA): RNAs that guide the insertion or deletion of uridine residues.
- Ribonuclease P (RNase P): Ribonuclease P is a type of ribonuclease which cleaves RNA. Acts as a catalyst in the same way that a protein-based enzyme would.
- Regulatory RNAs:
- Micro RNA (miRNA): A small non-coding RNA molecule (containing about 22 nucleotides) found in plants, animals and some viruses, that functions in RNA silencing and post-transcriptional regulation of gene expression.
- Small interfering RNA (siRNA): A class of double-stranded RNA molecules, 20-25 base pairs in length. By degrading mRNA after transcription, it interferes with the expression of specific genes with supplementary nucleotide sequences.
- Piwi RNA (piRNA): The most abundant class of small non-coding RNA molecules expressed in animal cells. piRNAs form RNA-protein complexes through interactions with piwi proteins.
- Trans-acting Small Interfering RNA (tsiRNA): A class of small interfering RNA (siRNA) that represses gene expression through post-transcriptional gene silencing in land plants.

RNA based technologies

RNA-based technologies are an essential toolkit for plant genomics functionality. More recent technologies have the potential to target RNA of a specific gene for alteration or silencing. Based on the gene target, RNA based technologies are categorized as:

Primitive gene silencing approach: RNAi : Advanced RNA based technologies: amiRNA, atasiRNA, TM, STTM, MicroRNA sponges,gRNA / Cas9

Primitive gene silencing approach: RNAi:RNA interference (RNAi) is a biological process in which RNA molecules inhibit gene expression, typically by destroying specific mRNA molecules. RNAi/small RNA-based gene silencing is extremely useful and has become a powerful approach to functional genomics, especially when genetic mutants are unavailable or not feasible. Depending on nature and structure of intermediate precursor of RNA molecules, sRNAs can be broadly grouped into

- **siRNAs**
- **miRNAs**

siRNAs: Long dsRNA precursors generated from exogenous dsRNAs, transposons, and viruses sRNAs through the action of RDR2 (RNA dependent RNA polymerase 2). dsRNA is processed by DCLs (Dicer-like) into many siRNA duplexes, which is subsequently methylated by HEN1(Hua Enhancer 1) protein. Methylated mature siRNAs are finally recruited into RISC (RNA Induced Silencing Complex) and guide degradation of target mRNAs.

miRNAs: Primary miRNA (pri-RNA), produced from MIR genes by RNA Pol II, is diced into pre-miRNA by DCL1. DCL1 and other accessory proteins further process Pre-miRNA into 21–24 nucleotide duplex miRNA. Duplex miRNA is methylated by HEN1 into mature miRNA duplex and transported to the cytoplasm through HASTY transporter. Guide strand of mature miRNA gets associated with RISC consist of AGO1 (Argounate), which has a catalytic domain and guide RISC to target mRNAs leading to either target cleavage or translation repression. However, Primitive gene silencing approach has several limitations such as in a dsRNA construct each IR (Inverted Repeat) that founds dsRNA needs to be 300-800 bp long for effective RNAi or gene silencingsiRNA species and a much high probability of causing "off-target" effect (silencing of the unintended gene) or transitive silencing (spreading the silencing to regions outside the inducer sequence).The degrees of silencing of target genes via dsRNA are difficult to regulate.For overcome those problems, several specific technologies for functional genomics of small RNAs have been developed.

Advanced RNA based technologies: RNA-based technologies, along with their development and practical genomic applications of plant coding and non-coding genes,emphasizes on artificial microRNAs (miRNAs), Artificial/synthetic trans-active siRNA (atasiRNA/ syn-tasiRNA),Target mimicry(TM),short tandem target mimics (STTMs),miRNA sponge (SP),and CRISPR/Cas9(Clustered regularly interspaced short palindromic repeats (CRISPR/ Cas9).

Artificial microRNA (amiRNA): Artificial microRNA (amiRNA): A customized 21-mer small RNA artificially made from an endogenous precursor miRNA (pre-miRNA), which is generated by the endogenous miRNA pathway.This concept was validated in a study and commercialized to develop the virus-resistant transgenic Arabidopsis plants.

Mechanism: Designed amiRNA is inserted into endogenous miRNA precursor by replacing miRNA/miRNA* sequence with respective amiRNA-amiRNA* nucleotides. This pre-amiRNA is processed by a series of DCL1 slicing events to generate mature amiRNA/amiRNA* duplex. One strand of amiRNA gets incorporated into RISC and guides RISC to inhibit target mRNA expression either by mRNA translation inhibition or degradation of mRNA.

Artificial/synthetic trans-active siRNA (atasiRNA/ syn-tasiRNA): Artificial/synthetic trans-acting siRNAs(atasiRNAs/syn-tasiRNAs) can also be used as an alternative to induce specific gene silencing in plants.Specially designed 21-mer small RNA artificially made from the tasiRNA pathway using modifiedendogenous transactivesiRNA (tasiRNA) precursor, such as TAS1 and TAS3. The atasiRNA / syn-tasiRNA are designed and generated to target the silencing of any gene or gene family of interest.Specially designed 21-mer small RNA artificially made from the tasiRNA pathway using modified endogenous transactivesiRNA (tasiRNA) precursor, such as TAS1 and TAS3. The atasiRNA / syn-tasiRNA are designed and generated to target the silencing of any gene or gene family of interest.

Mechanism: Pri-tasiRNA transcript is first transcribed from genomic TAS locus, cleaved by miRNA through AGO1, double-stranded through theSGS3 and RDR6 cooperative operation, diced to 21-nt siRNA, and HEN1 methylated. The 21-nt siRNA then directs the target transcript to sequence-specific degradation. AtasiRNA enables simultaneous silencing of several different target mRNAs

Target mimicry(TM): a phenomenon in which a non-coding RNA, with a non-cleavablemiRNA binding site, imitates and competes with the RNA to bind to amiRNA which, Also, it gives miRNA goal defence by sequestrating the miRNA away from goal. This phenomenon first was ascertained in Arabidopsis where the non-coding gene INDUCED BY PHOSPHATE STARVATION1 (IPS1) binds from its target, PHO2, a putative ubiquitin-conjugating enzyme E2 24, to and sequesters miR399

Short tandem target mimic (STTM): Based on the TM approach, a modified technique has recently been developed, STTM technology, which targets specific endogenous small RNAs for degradation in plants, and which is useful in knocking down the expression of miRNAs of an entire family. An artificial RNA structure has two miRNA binding sites that are linked by an RNA spacer of 48– 88 nt. STTMs can bind to target miRNAs without being cleaved by them. STTMs inactivate miRNA activity by degrading or sequestering miRNA away from its target gene transcripts.

STRUCTURE OF TTM

miRNA sponge (SP): The adapted SP technology for plants contains many more (up to 15) copies of miRNA binding sites that contain mismatches at the cleavage site to make them effective in knocking down the expression of target miRNAs. The higher complementarily of SPs than TMs to their target miRNAs may also result in a better binding and silencing efficiency in blocking miRNAs. SPs use many miRNA binding sites linked by a short (4 nt) untested spacer

Mechanism: Designed a miRNA is inserted into endogenous miRNA precursor by replacing miRNA/miRNA* sequence with respective amiRNA-amiRNA* nucleotides. This pre-amiRNA is processed by a series of DCL1 slicing events to generate mature amiRNA/amiRNA* duplex. One strand of amiRNA gets incorporated into RISC and guides RISC to inhibit target mRNA expression either by mRNA translation inhibition or degradation of mRNA.

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Mechanism: Generation of miRNA sponges depend on whether one, two or more miRNAs need to be targeted simultaneously with a single sponge construct. For this oligonucleotide, the approach can be used. For the oligonucleotide duplex approach, oligonucleotides are designed with two identical MBS (miRNA antisense binding sites). Each MBS is the antisense sequence of miRNA with a central mismatch at position 9-12 of the miRNA sequence (Bulge). This bulge is created by deletion of one nucleotide and changing the remaining three-nucleotide. A short 4-6 nucleotide sequence separates the two MBS.

Clustered regularly interspaced short palindromic repeats (CRISPR/ Cas9): Cas9 has now been modified to function for wide-ranging applications in eukaryotic cells including genome editing for gene mutation and modification transactivatingcrRNA (tracrRNA) for function in bacteria. Cas9 has now been modified to function in eukaryotic cells for wide applications, including genome editing for gene mutation and modification. Cas9 can also be controlled by transcriptional activation and suppression to control gene expression.

A diverse set of CRISPR-associated (cas) genes encode the proteins needed for the acquisition of new spacer sequences (Stage 1), CRISPR RNA biogenesis (Stage 2), and target interference (Stage 3). Each CRISPR locus consists of a series of direct repeats separated by single spacer sequences acquired from invading genetic elements (protospacers). A short motif flanks Protospacers Called the adjacent protospacer motif (PAM, * *) which is located in international DNA on the 5th (type I) or 3rd (type II) side. Long CRISPR transcripts are processed through distinct mechanisms into short crRNAs. A CRISPR-specific endoribonuclease in type I and III systems cleaves upstream eight nucleotides of each spacer sequence. In type III systems, an unknown mechanism trims the repeat sequence on the crRNA 's 3 range end. A trans-acting antisense RNA (tracrRNA) with complementarity to the CRISPR RNA repeat sequence forms an RNA duplex recognized and cleaved by cellular RNase III in Type II systems. This intermediate cleavage is further processed at the 5th end resulting in an approximately 40-nucleotide.This intermediate cleavage is also processed at the 5-point end resulting in an approximately 40-nucleotide crRNA mature with an approximately 20-nucleotide 3-point—the mature crRNA associates with one or more Cas proteins in each system to form a surveillance complex. Type I systems encode a Cas3 nuclease, which may be recruited to the surveillance complex for target binding. Some Type I systems have identified short high-affinity binding sites called the seed sequence, and genetic experiments suggest that Type II systems have a seed sequence at the 3 ends of thecRNA spacer sequence.

Comparison of Short Tandem Target Mimic (STTM) Technology with Target Mimic (TM) and Sponge (SP)Technologies: Endogenous IPS1 (INDUCED BY PHOSPHATE STARVATION 1) backbone-based TM technology showing the bulge (NNN), wobble (:), and mismatch (X) between miRNA and the miRNA binding site on the non-coding IPS1 RNA. (B) The improved STTM technology based on TM, showing a stronger interaction between the two miRNAs and the two miRNA binding motifs that are linked by a 48–88 nt spacer. The complementary regions show only bulges (NNN) with no wobbles/mismatches (C) The SP technology shows many copies (4–15) of miRNA binding sites with central mismatches (XX), which are linked by many (3–14) 4 nt spacers between 4–15 miRNA binding motifs.

Distinctions between CRISPR RNA-guided silencing systems and RNAi: Foreign DNA is integrated into the CRISPR locus in CRISPR systems, and long transcripts from these loci are processed by a family nuclease CRISPR-associated (Cas) or RNase III. The short CRISPR-derived RNAs (crRNAs) assemble with Cas proteins into large

surveillance complexes that target the destruction of invading genetic material.Long double-stranded RNAs are recognized as foreign in some eukaryotes, and a specialized RNase III family endoribonuclease (Dicer) splits these RNAs into short-interfering RNAs (siRNAs) that direct the immune system to invade RNA. PIWI-interacting RNAs (piRNAs) are transcribed from repetitive genome clusters often contain copies of retrotransposons and act primarily by restricting Transposonmobility.piRNA biogenesis has yet to be fully understood. MicroRNAs (miRNAs) are also expressed on the chromosome, and primary miRNA transcripts form stable hairpin structures tare processed sequentially (shown in red triangles) by two endoribonucleases (Drosha and Dicer) of the RNase III family.miRNAs do not participate in genome defence but are significant regulators of endogenous gene expression.

Like crRNAs, eukaryotic piRNAs, siRNAs and miRNAs associate with proteins that facilitate complementary interactions with invading nucleic acid targets. In eukaryotes, the Argonaute proteins pre-order the 5′ region of the guide RNA into a helical configuration, reducing the entropy penalty of interactions with target RNAs. This high-affinity binding site, called the 'seed' sequence, is essential for target sequence interactions. Recent studies indicate that the CRISPR system may use a similar seed-binding mechanism for enhancing target sequence interactions. **Application:** Those technologies have been exploited for the improvement of agronomic performance and nutritional value in various

Plant growth and development: The implication of those technologies in identifying the genes and transcription factors regulating growth and development processes of plants has flourished in recent past.Those approach has been successfully employed in understanding the molecular mechanism of flowering and associated genes, for instance, FT (Flowering Locus T) of *Arabidopsis.* In addition to determining the precise role of the flowering regulators, those have helped in developing specific knockdown lines of many growth unrelated genes, albeit they are significantly contributed to the growth and development of plants. Identification of involvement of heat shock proteins (HSPs) in growth and development. HSPs are known to play a crucial role in protein folding and response to various stresses in plants. Their requirement in chloroplast development was identified through amiRNA mediated silencing of *cpHsc70-1* and *cpHsc70-2*.] Male sterility is often considered as a useful agronomic trait for reducing self crossing. Complete male sterility of pollen was reported by targeting anther-specific TBP-associated factor genes (*SmTAF10* and *SmTAF13*) in *Solanum melongena* using those technologies.

Crop improvement : To feed continuous increasing global human population, the development of new crop varieties with increased engineering has been successfully proven its worth productivity is highly needed. More importantly, application of those technologies mediated gene silencing has also been exemplified in several reports, even in modifying the favourable agronomic traits of crop plants through manipulation of gene expression considering crop plants, the silencing of endogenous genes like phytoenedesaturase (*pds*), spotted leaf 11 (*Spl11*), and elongated uppermost internode (*Eui1*) was achieved through amiRNA technology in rice. The reduction in *Eui1* expression is thought to be one of the beneficial aspects of improving rice grain quality. In an attempt to increase the grain quality and economic value of rice, starch branching IIb (*SBEIIb*) gene was targeted through those technologies. Rice transgenic lines were expressing amiRNA against *SBEIIb*produced a more extreme starch phenotype which consists of an increased proportion of long amylopectin intermediate chains that is a demanding quality of rice grains. Similarly, betaine-aldehyde dehydrogenase (*BADH2*) in rice inhibited 2-acetyl-1-pyrroline (*2AP*) which is the principal compound responsible for grain fragrance. Interestingly, rice genotype having an aroma in grains was developed from non-fragrant variety by reducing expression of *BADH2* using amiRNA.The development of wheat streak mosaic virus (WSMV) resistant transgenic lines of wheat is another remarkable success story of amiRNA approach. WSMV is a persistent threat to wheat production and causes significant loss of crop every year. Fahim et al. (2012) have used a unique strategy, in which a polycistronic five arms of miR395 precursors, known as FanGuard (FGmi395) were utilized to target five distinct regions of the virus genome, and consequently, transgenic plants became immune to WSMV.A report described that suppression of genes involved in fatty acid biosyntheses, such as fatty acid desaturase 2 (*FAD2*), fatty acid elongase (*FAE1*) and fatty acyl-ACP thioesteraseB (*FATB*), led to the elevated seed oil compositionin *Arabidopsis*).

Elucidation of gene function in metabolic pathway: One of the most notable applications of amiRNA is to elucidate the function of any candidate gene in a short time as compared to conventional methods. Those approaches have successfully been applied for modulating flavonoid biosynthesis through degrading *NtFLS*(flavonol synthase), a key structural gene of the flavonoid biosynthetic pathway, and confirmed the role of flavonols in providing insect resistance. Transgenic tobacco plants expressing both *AtMYB12* and *amiFLS*miRNA transgenes displayed deep red flower colour and reduced rutin content in contrast to the white flower of *AtMYB12* expressing transgenic plants. This study provided evidence related to the insecticidal property of flavonols, especially rutin.

Biotic stress tolerance: Environmental stresses such as heat, cold, drought, salinity, redox stress and pathogen attack adversely affect plant growth and crop yield. Amongst common biotic stresses, different virus borne diseases are considered as major threats to crop production. They are responsible for the huge loss of economically important crops every year around the world. Studies indicate that endogenous miRNAs-mediated gene silencing is one of the mechanisms which potentially contribute to prevent virus invasion in plants. Those technologies have been successfully implemented to develop transgenic *Arabidopsis,*turnip, tomato, tobacco lines resistant to plant virus. Besides targeting viruses, deregulating the endogenous defence-related genes of the host can be another way for developing disease resistance in plants. Rhg1 was identified for soybean cyst nematode resistance in soybean. Conversion of dominant allele XAL3 into recessive xal3 allele through tissue-specific resulted in dominant traits bacterial resistant in transgenic rice.

Abiotic stress tolerance: Abiotic stresses like heat, cold, and drought comprise the significant challenges for plant growth. These stresses affect the growth, development and productivity of plants. Role of heat shock factor 1 (*HSF1*), a key regulator of thermotolerance in *Chlamydomonas*, was demonstrated using amiRNA. It is reminiscent from several studies that C-repeat binding factor (CBF) proteins play very crucial roles in cold tolerance of plants, and regulation of *CBFs* are believed to be under the tight control of MYB14 transcription factor. This interaction has been revealed by knocking down *AtMYB14* expression, which caused higher *CBF* expression and eventually increased the freeze tolerance. Silencing of another nuclear cap-binding protein, CBP80 in a potato (*Solanumtuberosum*) cultivar throughamiRNA resulted in improved drought tolerance in transgenic lines.

CONCLUSION

RNA-based approaches such as amiRNA, atasiRNA, Target mimicry, STTM, and gRNA / Cas9 hold enormous potential to study gene functions by knocking down, knocking in, or upregulating gene expression.This RNA – protein-interacting components can be improved by engineering a greater protein/enzyme partner, not only by altering the RNA partners but also by utilizing their biogenesis pathway components. These new tools strengthen the evaluation, and the use of substantial genomic information coming from post-genome studies in several species of plants performs a remarkable role in the assessment of plant biology and crop genetic advancements. Together by the use of constitutive, inducible, or tissue-specific promoters, these dynamic applications will analyze any desired genes or gene networks for their functions. Future developments must focus on efficiency, accuracy, simplicity, and reliability for the application of these technologies.

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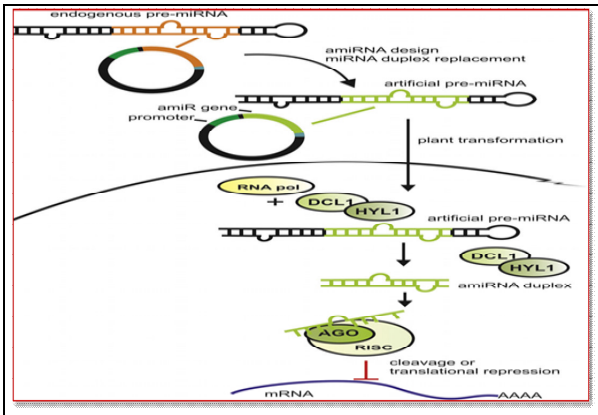

Figure.1.Artificial microRNA (amiRNA)

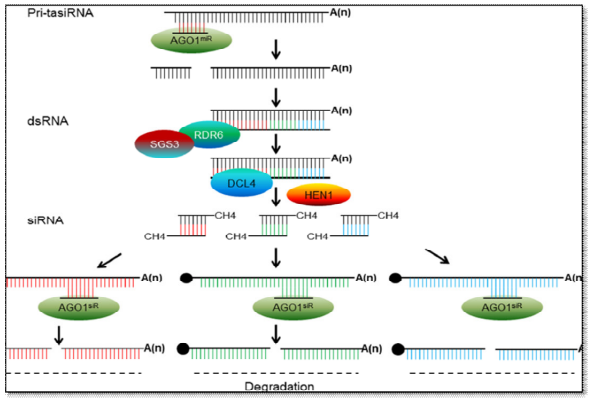

Figure.2. Artificial/synthetic trans-active siRNA (atasiRNA/ syn-tasiRNA)

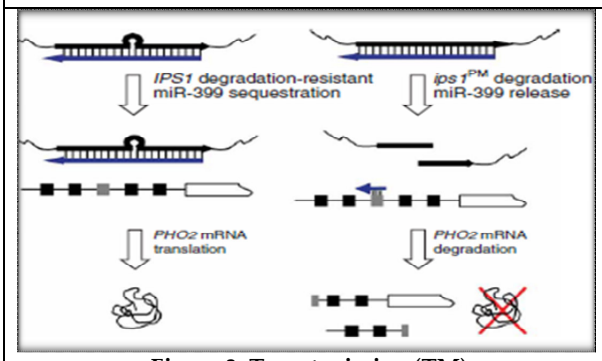

Figure.3. Target mimicry(TM)

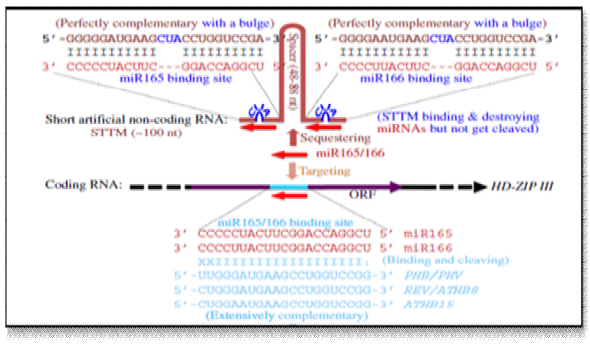

Figure.4. Structure of STTM

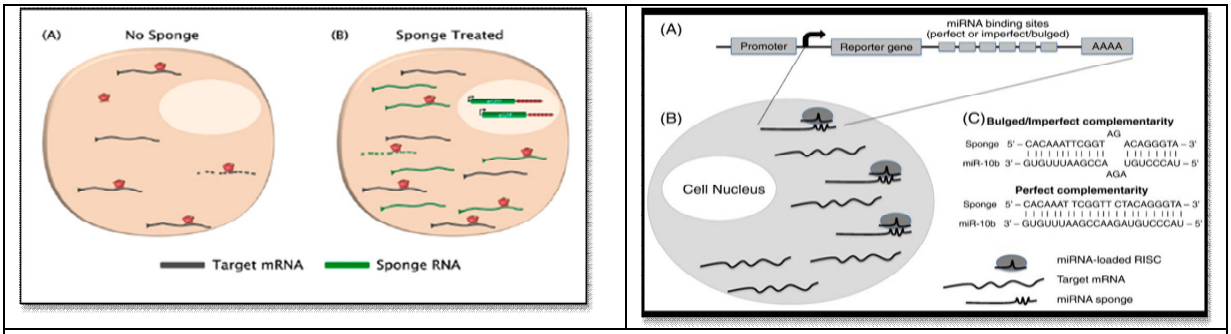

Figure.5. miRNA sponge (SP)

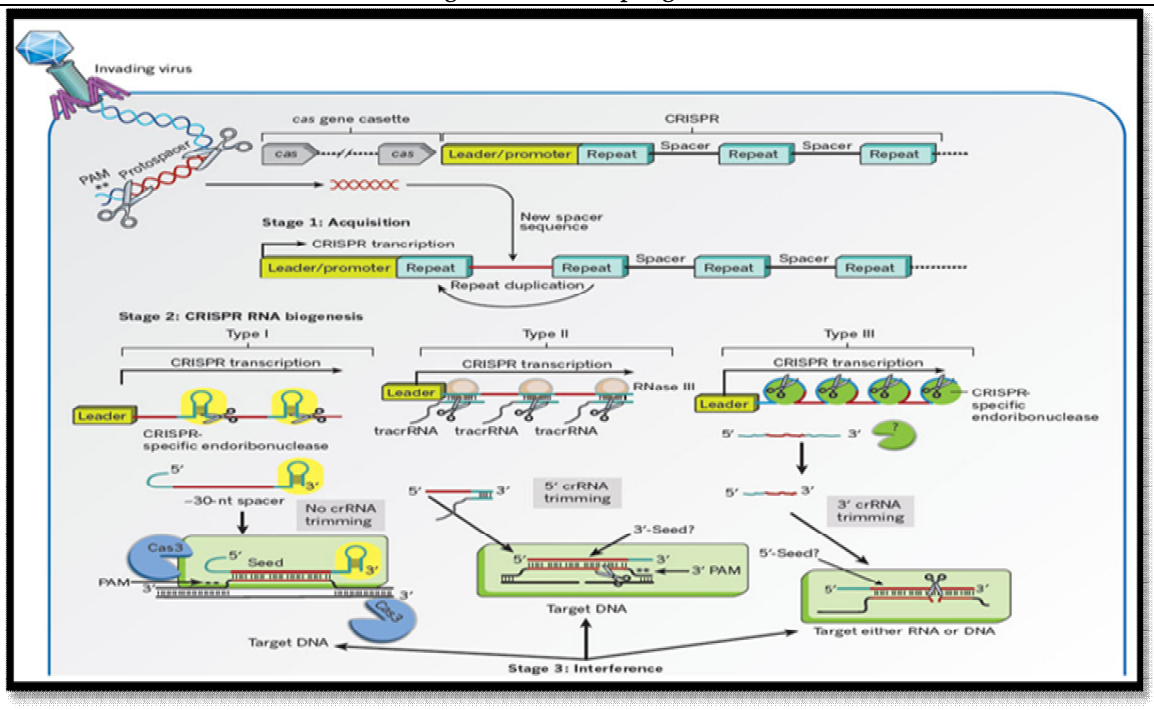

Figure.6. CRISPR/ Cas9

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RESEARCH ARTICLE

Exploring the Classical Language: Odia – a Historical Linguistic Approach

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ABSTRACT

Language is boundless and immeasurable. To apprehend a language to its core and to stumble upon the facts associated to it, are the bigger challenges that a language study involves. Commonly it is said that language comes from a place. But practically, language comes from the people who are a part of the place. A language stays in a region, dignified, when its people maintain its ethnicity in all ways. Odia, the language of the land of Odia's or the state Odisha, holds an extensive history coinciding the culture, politics, media and literature. Despite the fact that Odia language is widely accepted at various levels, there lies a certain inhibition in the modern day studies as to what is the position of the language at any recognised level. All the apprehensions were answered when Odia language bagged the Classical Language status in 2014 alongside five other classical languages of India. Language not only resides in the form of textbooks but also in forms of dance, music, sculptures and archaeological entities. While the language studies have surveyed Odia upon various levels, it is equally important to study the language from a closer prospect. This paper tries to encapsulate the history of the language, its rise, the current status of the language and the possible efforts that every linguist or language aspirant needs to think about to promote all aspects of the language.

Keywords: Odia, classical language, history of Odisha, language maintenance

A Brief Social History

The period of globalization demands a change in every culture and there isn't any exception from the respect of this process. Culture is one important element of the society because it adds social, physical, psychological and rational identities to the people living in it. The amalgamation of culture with globalization underlines many meaningful effects of changes that a society has been through. Talking of Odisha and its cultural elements, Odia is a language

from the history. It comes from the Eastern Indo-Aryan language group and primarily spoken in Odisha. Over 33 million people speak Odia. It is derived from Sanskrit and different languages comparable to Odia including Bangla, Assamese, Maithili, Magahi, and Bhojpuri. Indian states such as Jharkhand, West Bengal, Andhra Pradesh, and Gujarat also include a tremendous amount of Odia speakers. Specifically in the town of Surat, Gujarat there is a widespread Odia community due to immigration works in the diamond polishing and fabric industries. Although Odia is the mother language of Odisha, Telugu, Bengali, and Hindi are also spoken in this state. Internationally Odia is spoken in the United States by a diverse number of speakers and there are several organizations run by people that uphold the culture and language overseas. These societies help in maintaining the culture and spreading it with time. Reportedly, Odia societies are located in Maryland, New York, Illinois, Virginia, Michigan, New Jersey and currently spreading around the world to Singapore, Canada, and Kuwait.

Statistically Odisha is said to be a neglected state of India. People of Odisha, through the time, have survived with limited funds and inadequate support of healthcare, research, etc. Such factors have caused limitations in communication in addition to loss of necessary language studies and services. Due to this, research is few in number which makes it difficult to assess the language history and its development. Despite all odds, Odia becomes the first language from the Indo-Aryan linguistic group, the Sixth Classical Language of India. Also, Odisha became the first State under the British to be linguistically organized.In a span of ten years, i.e. from 2004 to 2014, a total of six languages were titled as Classical Languages. India being a plethora of languages that have ancient & historical originality, demands high attention. In cue with this, Odia received a positive response for being included in the classical language list in February 2014 for it has its own independent tradition and literature. It is reported that the earliest inscription in Odia was seen in 1051 AD. The language has many popular variations like Sambalpuri, Baleswari, Berhampuri, etc.

The Rise of the Language

Digitalisation of Odia: The Odia documentations exist from more than 5000 years back which is now a major part of Odisha. It hails from the Kalinga kingdom and the pre-Kalinga civilisation. The cave paintings in Gudahandi & stone inscriptions of Hatigumpha in Udayagiri caves are important sets in the history. More than the caves, there were sets of writing found in the age. The *64 Sidhapada* i.e. the Buddhist poets, wrote spiritual verses in Pali (1) language. There were inscriptions notably on bronze plates which came to be known as *Tambapata* and the ones on palm leaves were known as *Talapatra(2).*

From left- ***Talapatra and Tambapata:*** Odia has travelled from the age old legacies to the times of internet where the details are being digitalised in order to circulate them worldwide. New age reading tools such as e-books and e-magazines were taking their stands in the process. While all other languages had already made strong presence on internet, it took Odia almost a decade to be feasible in order to reach every keyboard. The reliable fonts being used then were Akruti, Leap Office, Shreelipi, etc. The major setback of these fonts is that they consist of Latin characters which results in difficulty to read & reuse if sent to an external system. The documents become incompatible most of the times. To breach the error, Unicode was launched in 2000. This advanced version has both Latin and Odia characters and can be universally accessed.

Due to a common platform in input systems, the Odia daily's started growing periodically. At present there are around 100 newspapers being published in Odisha from all regions. The realization that news and archives are of more commercial value than literary writings, helped in the growth of paper industry. It benefited the language. People no more used pirated software for the fonts. Soon Odia started domineering in the academics world where different categories of books were published. This invited writers, poets and publishers to work more towards the language. The advent of Odia content websites began with Odia Wikipedia (or.wikipedia.org), the largest Odia online encyclopedia with over 8,000 articles. Useful odia books for the community like classic literature, inscriptions, scriptures, lexicons, journals & research papers were periodically posted and updated in this community website. The page has both volunteers and contributors who can edit content or contribute to the page as well as maintain

authenticity levels. *Srujanika*, a Bhubaneswar based organization along with *National Institute of Technology*, Rourkela and *Pragati Utkal Sangh*, Rourkela has scanned over 760 Odia books. Out of which over 200 books are hosted in "Open Access to Odia Books (OAOB)" and at oaob.nitrkl.ac.in. Organizations like *Manik-Smrutinyas* and *Institute of Odia Studies and Research* have re-licensed books of noted authors for free, commercial distribution. Majority of magazines, publishers and university or government organizations are requested and asked to grant free access so as to promote research & development with the help of these sources.

Research and Education: The state government sanctioned 25 acres of land specifically for setting up the Odia University at Satyabadi(2) (Sakhigopal) of Puri district. It is the second language university after Jagannath Sanskrit Vishvavidyalaya. The aims of the universities include facilitating research in language time to time and its promotion. But the fact remains, that there is a lack of educationalists and teachers for Odia language. Around 50 percent of teaching posts in Odia are lying vacant in all general colleges. The existing teachers however are struggling with their position to produce research work due to insufficient resources & opportunities. Currently Post Graduate degree in Odia is offered by reputed varsities like Utkal, Berhampur, Sambalpur, Gangadhar Meher, North Odisha, Rama Devi, Ravenshaw and Fakir Mohan University. The total number of sanctioned positions is 56 which include Professors, Associate Professors and Assistant Professors. The minimum requirement stands as: 1 Professor, 2 Associate Professors & 4 Assistant Professors. But on the whole, as many as 28 posts are still vacant for the same. At Fakir Mohan University the posts of Professor and Associate Professors have been lying vacant for a long time. At GangadharMeher University, the department runs with two Associate Professors. Utkal University, Ravenshaw University and Berhampur University still lack Professors which hampers the teaching & supervision to some extent. In addition to this, the Higher Education Department of Govt. of Odisha reports that 60 percent of Odia teaching posts are vacant in higher secondary schools, intermediate and degree colleges.

For a long period i.e. from 1998 to 2012 there were no scholars in Odia. Strong academicians who then passed the course had started retiring. The gap that got created still affects the fraternity. To put this logically, if someone completes post graduate degree now and gets awarded doctoral degree or qualifies the National Eligibility Test, they would be eligible to teach but it is quite a process in matters of time. Until then the posts aren't likely to get filled up too. With time, the students' outlook towards pursuing Odia language as a career is changing and meritorious students are now coming forward. Earlier if a student did not get any honours they'd opt for Odia, otherwise not. This will eventually change the employment scenario in the subject. In today's situation, the approach towards advanced studies is something that the subject needs. The concepts of translation, critical analysis & research, linguistics stand important for mining up the ancient Odia texts.

Political Movement or Cultural Awakening?

Odisha acquired its position as a state on the basis of the Odia language. But in general the government hadn't taken any active participation to promote the language due to lack of participation of its people. This is when the Odisha Bhasa Andolan was founded. The movement encompasses that Odia must be a household language for offices, business, courts of law, educational hubs, etc. the language of the state should be the language of the people as a whole. Nabakrushna Choudhury, the then Chief Minister of Odisha brought up the *Odisha Official Language Act* in 1954 to make sure that a process starts in order to globalize Odia. Odia not only should be an official language but a domestic language too. It should be common in households, among people and children, in a way such that there's no generation gap in regard to knowledge and origin of language. It is seen that Odia in western Odisha has Hindi predominance, southern Odisha has Telugu and northern Odisha has Bengali dominance. On the web, there is a fusion of Odia, English and Hindi. Odia as a language demands preservation, protection and propagation. In due with the 1954 language act, people around the state started building pressure on the government claiming that four crore Odias need to see their language alive. None other than the political parties could sack in pressure for this. *This was not a political movement against anyone but a cultural awakening!* Saving Odia became the concern of common man.
November 23rd was officially declared as the "Bhasa Divas" since it is the birthday of the father of the Language Act, Nabakrushna Choudhury. The consents and declarations from the government in the following period established

strong foundations in the minds of people. Modern schools and educational institutes started working on introducing Odia studies under the head Regional Language Studies. Central budgets were roped in and private sectors soon started accepting the implementation. The unintentional conspiracy of traditionalism vs. modernism that however started mentally among us weakened the roots of our mother language. Somehow, modernity of the world came to its rescue.

As a Medium of Instruction

India, the multilingual country functions with 1576 mother tongue languages(6), 22 official languages (7)and 13 different administrative languages. The National Curriculum Framework (NCF) – 2005 argue that the most suitable medium of instruction in any case is the mother tongue. The thoughts and expressions on either side can be effectively achieved. The education through mother tongue idea also promotes multilingual education since India is largely seen having cultural diversities. Cummins'(8) three language formula promotes multilingual communicative abilities in a country like India. This three language formula says that instructions in L_1 (first language) provides a sound base for the development of proficiency in L_2 (English) which means that the cognitive and conceptual skills can migrate from a native language to English. Thus focus was laid on the fact that children should be mastered with L_1 or the mother tongue first as it is a 'pre-existing knowledge base'.

Measures taken

The Right of Children to Free and Compulsory Education Act (RTE) of Article 21-A regulated in 2009 facilitates free and compulsory education to children within the age group of 6 to 14 years as a right. Every child has the right to free, qualitative, elementary and equitable education. The RTE Act became active in Odisha on 1st April 2010. In this light, he Government of Odisha undertook the responsibility to promote Odia language and culture, bifurcating the Tourism and Culture department in 2017. A dedicated wing was set up and named as the 'Heritage Cabinet' to manage and protect the monuments, ancient temples, scriptures and moreover the language. The cabinet demanded all shops and business places to build/rebuild their nameplates and signboards in Odia language. It was also prescribed that there would be punishment for non-abidance of such rules. On academic grounds, students are given ample opportunities. Students will be facilitated to pursue research in Odia as per UGC pattern, fees of meritorious students will therefore be waived off. State level programs or national level conferences, workshops& seminars are increasing from time to time.

The next important aspect includes the problems faced by tribal communities. There was an inherent issue with acquiring their mother tongue as the tribal children faced language gap. The Multilingual Education Program (MLE) of the Government in 2007 regulated a few points for accelerating language learning in the minority communities. Some of the important measures are noted below -

i. The mother-tongue (MT) of tribal children will be used as the medium of instruction for the five years of primary education in the MLE program in Odisha for sustained impact on tribal children's educational achievements, high levels of proficiency in Odia and English.
ii. English is to be introduced as a language subject in the MLE program from Class III. The tribal languages may be used as language subjects in post-primary levels starting from Class VI.
iii. Candidates with fluency in the mother-tongue of the children as well as competency in Second Language (L_2-Odia) and Third Language (L_3-English) will be given priority for recruitment as teachers in the local MLE Schools. Separate advertisement will be issued for MLE teachers specifying knowledge of the target mother-tongue as an eligibility condition.
iv. Candidates from the community with lesser qualifications but target proficiency will be engaged on contract basiswith a condition of acquiring the required qualifications within a reasonably stipulated time.
v. Children belonging to at least three mother-tongue skills will be identified to start a pilot program for development of teaching-learning plans for a purpose.
vi. MLE program will be implemented with an emphasis on sound pedagogic principles under the guidance of experienced pedagogy experts.

vii. The pedagogy in MLE program must seek to balance between the languages and diverse cultural practices in a manner that can effectively challenge the positioning of some dominant languages and cultures, building a strong sense of identity and pride in children's own language and culture.

viii. Team Leaders of all the language groups in the MLE program will go through an Orientation Workshop on Preparation of Textbooks and Teaching Learning Materials (TLM) with focus on basic aspects of MLE, curriculum, pedagogy, language issues, cultural content and other considerations in material preparation for linguistic minority children.

ix. Language-based teacher training institutes will be established preferably in the tribal districts of the State. The MLE program will be tied up with *the* English Language Training institute (ELTI) for providing training in Third Language (L3-English) to the MLE teachers.

x. Assessment of children's competence level in curricular and co-curricular areas and activities will be made in their mother-tongue following the mode of Continuous and Comprehensive Evaluation (CCE). Besides curricular progress, the personal-social characteristics of children such as attendance, participation, classroom interaction, peer interaction etc. will be qualitatively assessed.

xi. Cumulative school report/progress cards will be prepared in the local language and shared with parents. The assessment outcomes will be reviewed in regular duster-level meetings in order to develop remedial measures and evaluate the impact of remedial intervention.

xii. MLE program will strengthen its research and development activities at different levels of the program. While at the State-level research is necessary to assess the overall functioning and the impact of MLE schooling, at the cluster level the teachers will be suitably oriented to conduct action research to bring improvements and innovations into the system at the grassroots level.

CONCLUSIONS

With the higher secondary schools across the State yet to implement the Government order to use Odia language in all official works, the Directorate of Higher Secondary Education (DHSE) recently asked the schools to execute the provisions under Odisha Official Language (Amendment) Act immediately. According to the Act, Odia has to be used in all official communications by the Government offices. But various offices including junior colleges and other educational institutions are yet to implement the order. While there should have been communication in both English and Odia languages in official work, most of the Government letters are being issued in English. In order to ensure its proper implementation, the State Assembly had passed the Odisha Official Language (Amendment) Bill, 2018 with penal provisions. In May 2016, the State Government had brought an ordinance to enforce the Official Language Act, 1954 for all communications. Despite having provisions of punishment for non-compliance and rewards for officials, it failed to encourage them for maximum use of Odia language.

The Chief Minister of Odisha had to face a number of speculated objections when these rules regarding implementation of Odia were made rigid. Criticism was blunt upon him for his lack of command in the language. While the people on and off their duties practiced to regulate Odia, the ruler of the state was satirized by various media channels and opposition parties. Nevertheless, the effects of the official act grew stringer with time. It also influenced the Tripura government to mandate the use of *Kokborok* language on all signboards, nameplates and notice boards. Similarly, the Telangana government announced *Telugu* to be put up on signboards and in 2015 *Kannada* was regulated in Karnataka for the same. Following this, there was a Cabinet Meeting held which was conducted in Odia. There were also incentives for employees and departments for the use of Odia. The improvements and reciprocations have been happening for more than a decade and has transformed to an invariably bigger picture.

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3. Odisha holds the record of having the largest number of palm leaf manuscripts (over 20,000)
4. "Satyabadi" is the land of famous Panchasakha (five comrades). In its honour, the Odia Varsity was decided to setup at Satyabadi
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Fig.1. From left- Talapatra and Tambapata

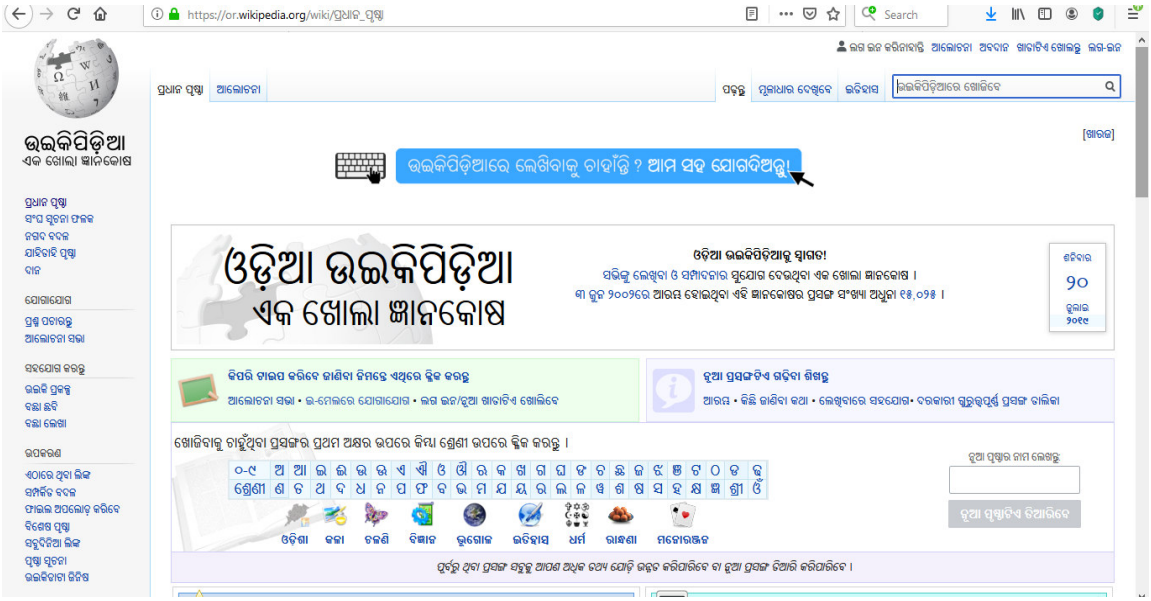

Fig.2. OdiaWikipedia homepage– or.wikipedia.org

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RESEARCH ARTICLE

Structural and Impedance Properties of Iron (Fe) based Ceramic

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ABSTRACT

The Fe based ceramic NdFeAsO was prepared by solid state reaction method. Tetragonal crystal has been confirmed at room temperature through X-ray diffraction technique. The complex impedance plots reveals presence of both bulk and grain boundary effects, and non-Debye type of relaxation process occur in the sample. The material shows the negative temperature coefficient of resistance (NTCR) behavior. The dc conductivity data of the sample obeyed Arrhenius equation. The activation energy of the sample was found to be in the range 0.46-0.88 eV.

Keywords: X-ray diffraction, Ceramic materials, Impedance study, Activation energy

INTRODUCTION

The iron (Fe) based ceramic NdFeAsO is one of family of layerd high temperature superconductor with transition temperature 50 K. The discoveries of iron-based superconductors (FeSCs) have been greatly emphasized by the researchers due to simultaneous existence of their superconductivity and magnetic properties, having a layered structure [1-8]. The Fe based $RFeAsO_{1-x}F_x$ of rare earth family having R=*Sm*, *Ce*, *Nd*, *Pr*, *Gd*, *Tb* and *Dy* compounds come under FeSCs having highest superconductivity transition temperature (T_c~54 K). In these compounds, superconductive properties may be manifested due to FeAs and R (O/F) layer in which former layer behave as superconductive planes and later layer serve as charge reservoirs [9-11]. Among these, the compound $NdFeAsO_{1-x}F_x$ materials have a layered tetragonal crystal with crystallographic axes $a = b = 3.962$ Aº and $c = 8.555$ Aº [12-15]. Realising the importance of layered FeSCs particularly its superconducting nature at some high temperature we have synthesized Fe based polycrystalline ceramic NdFeAsO and studied their structural and impedance properties at high temperature in order to have complete the systematic prospective.

Experimental

The ceramic material NdFeAsO was prepared by solid state reaction techniques from the pure oxides: Nd_2O_3, Fe_2O_3, As_2O_3 with high purity in a suitable proportion. The stoichiometrically weighed compound for a particular composition was blend in air atmosphere for 2 h and then in methanol for 2 h by using an agate mortar and pestle to get homogeneous mixture of the materials. The mixed powders were calcined at 1100°C for 5 hrs. The quality and formation of the calcined compound were checked through an X-ray diffraction (XRD) method at room temperature using CuK_α radiation (λ=1.54 Å). The calcined powder were mixed with polyvinyl alcohol (PVA) which was used as binder o reduce brittleness of the pellets and then pressed into cylindrical pellets using hydraulic press. The pellet was then sintered 1150°C for 6 h. The binder PVA burns off during this process of sintering. In order to have both faces flat and parallel, the sintered pellet was then polished with fine emery paper. The flat polished surfaces of the pellet were then coated with air drying conducting silver paste. The pellet was dried at 150°C for 2 hrs to remove moisture (if any) before taking any electrical measurements.

RESULTS AND DISCUSSION

Structural analysis

Fig.1 shows the room temperature XRD pattern of NdFeAsO. The XRD data of the prepared sample suggested the tetragonal crystal system and most of the peaks are well matched with the previous report **[16]**. There is a good agreement between observed and calculated inter planar spacing d is seen. The lattice constants of the selected tetragonal structure are refined using a standard computer program package "POWD" **[17]** and found to be a=3.9763 Å, c=8.6469 Å, c/a=2.174.

Complex Impedance Study

Complex impedance spectroscopy technique has been recognized as a unique, non-destructive powerful technique to characterize the transport properties of solids **[18].** Generally, the contribution of bulk, grain boundary and electrode effect in the materials can be evaluated by separating the real and imaginary components of the complex impedance parameters. These parameters may be calculated from the basic formalism as: $Z^*(\omega) = Z' - jZ''$, where $Z' = |Z|\cos\theta$ and $Z'' = |Z|\sin\theta$ and complex electric modulus as: $M^*(\omega) = M' + jM''$, $M' = \omega C_0 Z''$, $M'' = \omega C_0 Z'$, where ω is the angular frequency ($2\pi f$), $C_0 = \varepsilon_0 S / d$ is the geometric capacitance, ε_0 is the permittivity of the free space, S is the area and, d is the thickness of the sample.

Fig.2 shows the variation of real part (Z') and imaginary part (Z'') of impedance at different temperatures (100-200°C) in wide frequency range for the sample. A single semicircular arc is observed up to temperature < 125°C and two semicircular arcs are observed at moderate temperature >125°C. This shows that at low temperature (≤125°C), the electrical process of the sample is determined by bulk properties, whereas at high temperature the total electrical response of the composites is due to the contribution of both bulk and grain boundary effect. This indicates that, at low temperature, the localized relaxation due to bound charges predominates, and at higher temperatures, the relaxation in the sample has components from both a long range and localized relaxation.

The Nyquist plots also show the depressed semicircles whose centre lies below the real axis and exhibit non-Debye type of relaxation phenomenon in the compound **[19].** Further, it is observed that the bulk resistance decreases with increase in temperature which shows the negative temperature coefficient of resistance (NTCR) behavior. Fig.3 and Fig.4 shows the variation of Z′ with frequency at different temperature (100-450°C) for NdFeAsO. It is seen that the value of Z' decreases with increase in temperature and confirms the NTCR behavior as observed in Nquist plot. The Z' value decreases with increase in frequency for all studied temperature and merge at single frequency. The

merging of graphs at particular frequency may suggest the release of space charge. The merging of graphs takes place above 20 kHz.

Fig.5 and Fig. 6 shows the variation of imaginary part (Z″) with frequency at different temperatures (100-450°C) for NdFeAsO. From Fig. 5, It is observed that the magnitude of Z'' increases with increase in frequency and attains a maximum value at a particular frequency and then decreases. This trend has been seen clearly in the higher temperature region 125-200°C. The peak of Z'', indicates the presence of relaxation process in the materials. The peak value of Z'' shift towards higher frequency side with rise in temperature confirms the presence of temperature dependent relaxation process in the material. This may possibly the presence of small polaron at low temperature and defects at high temperature responsible for broadening. The merge of all Z'' curves at higher frequencies (irrespective of temperature) indicates the absence of space charge polarization [20-21]. From Fig.6, it is observed that in the high temperature region the merging of Z'' is also observed for low frequency region. The merging of Z'' exist upto the frequency 50 kHz and after that its value increases with increase in frequency irrespective of temperatures.

Activation Energy

The activation energy can be calculated using the Arrhenius relation [22] $\tau = \tau_0 \exp\left(-E_a / K_B T\right)$, where the symbols have their usual meanings. Here the relaxation time τ can be found out using relation $\tau = 1/2\pi f_{\max}$ where $f_{\max}$ is the maximum relaxation frequency corresponding to $Z''_{\max}$. The variation of τ with inverse of selected temperatures for the sample shown in figure 7. The values of activation energy calculated from the slope of the curves is found to be 0.88 eV. Also the activation energy can be calculated from variation of dc conductivity with inverse temperature. The dc electrical conductivity is evaluated from the impedance data using the relation, $\sigma_{dc} = d/SR_b$ where *d* and *S* are thickness and area of sample respectively, R_b is the bulk resistance. Fig.2 shows the variation of dc conductivity with inverse of temperatures (375°-475°C). It is found that the dc conductivity increases with rise in temperature for all the samples. The nature of the plot found to obey the Arrhenius relation $\sigma_{dc} = \sigma_0 \exp\left(-E_a / K_B T\right)$. The value of activation energy calculated from the slope of the plot and found to be 0.86 eV. These two values of activation energies are close to each other.

CONCLUSIONS

The iron (Fe) based sample NdFeAsO was prepared by a solid state reaction technique. The tetragonal structure at room temperature was confirmed through structural analysis. Impedance studies reveal the significant contribution of grain (bulk) and grain boundary effect. The bulk resistance of the material decreases with rise in temperature and exhibits NTCR behavior. The variation of relaxation time and dc conductivity of the material as a function of temperature exhibits Arrhenius type of behavior. The activation energy lies in the range 0.86-0.88eV.

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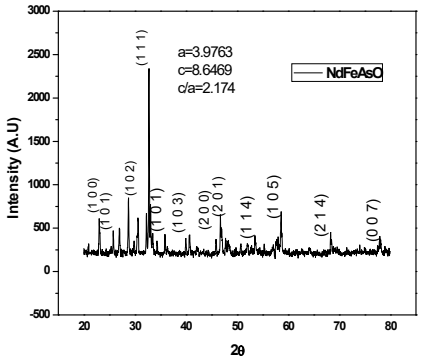

Fig. 1 X-Ray diffraction patterns of NdFeAsO at room temperature.

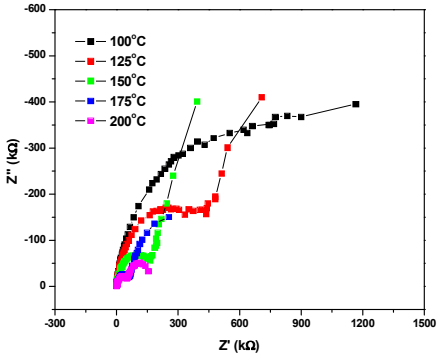

Fig.2 shows Nyquist plot (Z′ vs. Z") of sample NdFeAsO at different temperatures (100-200°C)

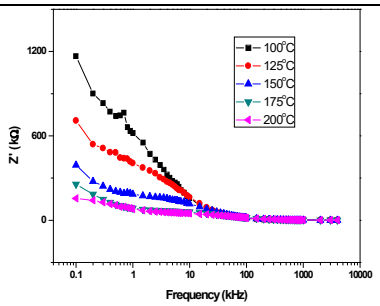

Fig.3 shows Variation of Z′ with frequency at different temperature (100-200°C) for NdFeAsO

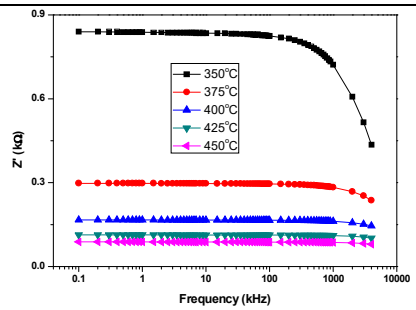

Fig.4 shows Variation of Z′ with frequency at different temperature (350-450°C) for NdFeAsO

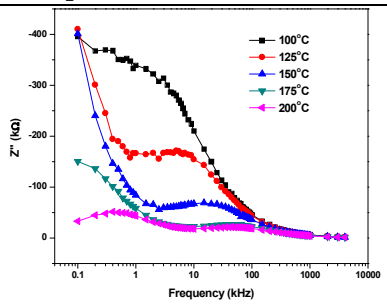

Fig. 5 shows Variation of Z'' with frequency at different temperatures (100-200°C) for NdFeAsO

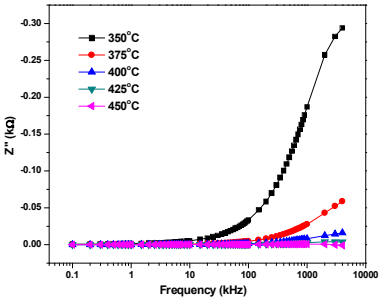

Fig.6 shows Variation of Z'' with frequency at different temperatures (350-450°C) for NdFeAsO

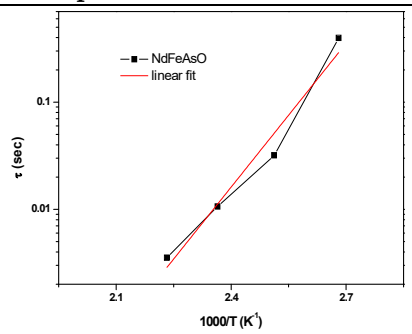

Fig.7 shows the variation of τ (calculated from impedance plot) with inverse of selected temperatures for NdFeAsO.

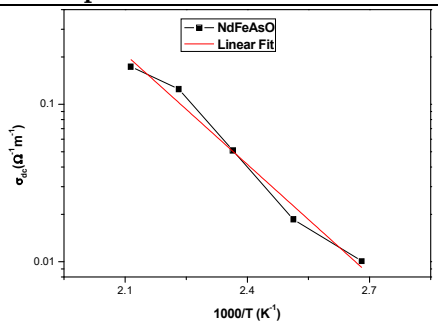

Fig. 8 Shows Variation of dc conductivity with inverse of temperature (375°-475°C) for NdFeAsO

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RESEARCH ARTICLE

Real-Time Slide Door Automation and Security System with RF Technology

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ABSTRACT

RFID otherwise known as Radio Frequency Identification is a quite fascinating technology available at our disposal for quite a time. It has been implemented for several applications in the near past. Applications like garment industry, item tracking in malls, production line tracking etc. its popular because of its low cost long life and reliability. It enables identification from a distance, and unlike earlier bar-code technology, it does so without requiring a line of sight. RFID tags have a unique ID than bar codes.Security is an essential parameter today, everyone and every thing is analysed on the measure of security first then its used or utilised. So many researchers have targeted RFID as source of security provider. When security is the question no industry, no home and no person is an excecption. Various control systems have been designed over the years to prevent unauthorized access. This article is focused on the application of RFID to the security of an automated slide door. As each RFID tag or card is associated with an unique identification code it is quite justified to use it as a security measure to access into a room. The slide mechanism is automated usind a high torque DC geared motor and chain arrangement. Access into the room is limited to specific person with RFID cards. Another level of security is implemented is the password protection system to initiate the security module upon system reset or power failure. This module enables us to enter the password through a 4x4 keypad. If the password is not entered correctly then the RFID cards cant have access. Since two way security is implemented its quite rubost and secured for implementing in a house or small office.

Keywords: Arduino Uno, RFID, Door Lock, keypad, LCD

INTRODUCTION

Security and safety become vital everywhere now. So a security system is a requirement for individuals and an organization for safety into the residents and property. For this reason, the multi-way access control system is proposed. This system can be implemented in offices and home premises. This system allows only the authorized users i.e. the users who enter the correct passcode or show the valid RFID tag, to enter the homes or office. Door security is used in many commercial, governments, and residential buildings. This type of security is known as smart locks where it limits the only person, who knowsan electronic password. There are different types of door locks based on security levels. There are also various types of door locks available in the marks in the various shapes, sizes, and designs.

LITERATURE REVIEW

Many of rhe related research papers are refered prior to designing this project so as to make this model a fill-in some gap in the reseach and validate the concept of the work. Few researchers have worked on the digital code locking system as a security measure in automobiles [1]. Even some have worked on the use of DTMF through GSM module and hardware arrangements as a security measure to door locking and un-locking system [2]. A model comprising of a GSM mobile, IR sensor, LPG sensor and Fire sensor is proposed that has a keypad interface to enter the password and access the room [3].

The use of RFID tags and strips doesnot end in appliance tracking, garment tracking and home security, it has also been used biological body tracking i.e tracking of birds and animals to record the feeding rates, incubation behaviour, pair formation, homing behaviour, prospecting behaviour by non-breeding birds etc. [4]. A model comprising of RFID, GSM, Keyboard and LCD connected to a microcontroller is used as a security module for giving access to authentic person only [5]. A hostel security system is proposed to ensure that, only registered hostel in-mates have access to the services provided. This system captures the card holder image and compares it with the registered databse if a match is found then access is granted else an alarm is raised [6]. A magnetic door locking system is proposed which can be accessed by RFID recognisation system.

They have used Arduino interfaced with the modules and connected to the PC to store relevant information as the system also records the access information in the computer [7]. A system comprising of Barcode scanner and RFID reader is used to create a match. If a match is found the student is allowed to leave else the student is detained [8]. Another simple system is encountered that uses an RFID tag to authenticate access to an entry point which closes after a specified time interval [9]. A security system implemented on a door with RFID tag reader and an interfaced SDcard is proposed where on authorised entry the controller saves the information in the SDcard and allows access through the door and parallelly the card holder information is displayed in the LCD connected [10].

Proposed Methodology

The controlling unit of this work is Arduino Mega. The other components are interfaced to this microcontroller. The door automatically opens when either the correct passcode is entered using the Keypad or valid RFID tag is placed near to the RFID reader. And the closing of the door is controlled through another passcode. The LCDs “Door Opened” and “Door Closed” when the door opens and closes respectively. In case of incorrect passcode or invalid RFID tag, the door remains closed and the LCDs “Wrong, try again”. The opening and closing of the door are controlled manually through the switches from inside the room. When the open switch is pressed, the door opens and when the close switch is pressed, the door closes. Two status LEDs are also used to show the validity of the user i.e. whether the user is authenticated or not to enter the room. In the case of correct passcode and valid RFID tag, the green LED glows, otherwise, the red LED glows.

As can be seen from the fig 1 from the flow chart, at first, the LCDs a message which welcomes the user and asks him to enter the passcode or show his RFID tag. Then the user uses any of the methods i.e. enters passcode using Keypad or uses a valid RFID tag to enter the room. In the case of the correct passcode or valid RFID tag, the door opens automatically. In the other case, the door remains closed, the user is asked to try again. Once the authorized user enters the room, he can close the door by pressing the close switch installed inside the room. Similarly, to come out of the room, he can press the open switch to open the door. The power source is connected to the microcontroller to give sufficient power supply for the smooth functioning of the project. The 4x4 Keypad and RFID are connected to give input to the microcontroller i.e. passcode is entered through Keypad and RFID tag is shown to the RFID reader. The LCD is connected to display each operation like "Enter Passcode or Show your Card", "Door Opened", "Door Closed" and "Wrong, try again".The status LEDs are used to show the status of the door i.e. whether the door is opened or not. In other words, it is used to show the validation of the user i.e. whether he is allowed or not to enter the room. In the case of correct passcode and valid RFID tag, the green LED glows, otherwise, the red LED glows. Relay is used to drive the DC Motor which in turn drives the door. Can also be closed from outside the room by entering another passcode through the keypad.

Arduino Mega

As we know that Arduino is a open sourse hadware and software. It has project and user community. Arduino boards uses different microprocessor and controllers. The board contains few no. of input, output pins , which is used to connect the pripheral devices.So here we have used Arduino mega because it has more no. of input output pins as compared to the other boards.

Frame

The frame shown in Fig 3 is made up of metallic bars with appropriate dimensions and is placed in a measured area. It has been made with the help of welding. The gears and motor are fitted on the frame with proper alignment. The chain is also properly aligned on the frame and connected to the door.

DC Box Gear Motor

The below shownin Fig 4 DC motor is used to open and close the sliding door of a classroom. When the DC motor moves in the clockwise direction it opens the door. Similarly, when the motor rotates in the anticlockwise direction it closes the sliding door. This motor is fitted with the above-shown frame. RFID comes with a Reader and Tag. They used RF technology to read and capture the pieces of information. Reader connected to the microcontroller when powers up, create an RF signalfor up to several feet. When Tags are brought nearer to the reader then it reads the unique ID.there are a variety of tags available in the market. They are active and passive. Passive RFID Tags are used for short-distance communication, usually 10 feet or less.The most commonly used RFID reader is the EM-18 reader module. This module has a built-in antenna that is used to power the RFID Cards and also extracts the information from the Card's microchip.

4*4 Keypad

This module is used to enter the password for the door security system. A keypad consists of set of swiches arranged in rows and columns. This type of keybard are known as Matirx Keypad.

Arduino IDE

It is the open sourse software which makes it easy to write, edit, compile, upload codes into the varities of Arduino boards. This is basically a integrated development environment which supports varities of Arduino based microprocessor. It has supported files for windows , Linux and Mac OS.

Simulation Results

The beneath figures show the constant usage of the RFID based Door mechanization and security System. This framework comprises of two different ways to computerize and make sure about the entryway. The two different

ways are 1) with the assistance of Keypad and 2)with the assistance of the RFID framework. At the point when the individual is going for the principal way utilizing 4*4 keypad, the individual who realizes the passkey can just have the approval to open the entryway. At the point when the individual is going for the second technique, then he/she should have an RFID tag without that he isn't permitted to open the entryway. The framework is structured so that in the event that the individual neglected to have the RFID tag, at that point he may straightforwardly enter the passkey utilizing the keypad and can go into the Room. In the board box, there is no choice to set or reset the secret key in light of the fact that to make sure about the room. So just those can alter the passkey who has a thought regarding the programming. The RFID labels are given to the concerned people who are utilizing that room, others are not permitted to go into the room without their earlier data. The continuous model structured is appeared in Fig 8. From the start, the client is approached to enter the password or show his/her card. At that point, the client utilizes any of the strategies for example enters a password utilizing Keypad or utilizations a substantial RFID tag.

Using the Keypad

Step1: When the correct passcode is entered using the keypad, it displays"Door Opened" on the LCD,and at the same time the Sliding door starts moving and the inturn opens the door.

Step2: When the passcode entered is incorrect, it displays "Wrong! Try Again" and the door remains closed

Step3: The door can also be closed by entering another password, which is set through the program.

Using RFID Technology

Step1: When a valid RFID tag is used, it displays "Door Opened", sliding door starts moving and opened the door, shown in fig 12(a).

Step 2: In the case of an invalid RFID tag, it displays "Wrong! Try Again" and the door fails to open whichshown in fig 12(b).

Using switch

The opening and closing of the door can also be controlled manually through the switches. Once the user has entered the room, he/she can come out of it by using the switches.shown in fig 13(a)(b).

Step1: When the Open switch is pressed, the door opens

Step2: When the Close switch is pressed, the door closes.

CONCLUSION

A secure door lock system or access control system has become necessary nowadays to prevent access to unauthorized users to the office and home premises for the security of our lives and properties. And RFID is increasingly used for security and access control applications. In this project too, we have successfully implemented an access control system using passive RFID. When the user puts the valid tag near the RFID reader, the door opens automatically, otherwise, the door remains closed. Alternatively, users can also enter the correct passcode using Keypad. Hence, this system provides more security as the entry of unauthorized users is restricted through two secure ways – Passcode or RFID tag.

This project can be further modified to an advanced level by adding the following features:

1. Resetting password
2. Retrieving the previous password

Which can be done by using a GSM Module and registered mobile number. When the administrator himself forgets the password he can reset the password wirelessly through a mobile phone.

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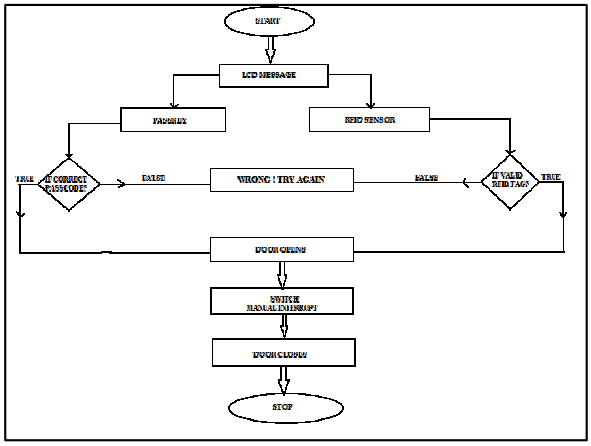


Fig 1: Flow Chart

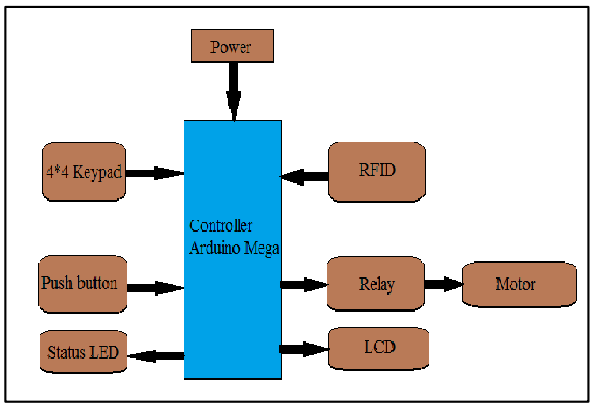


Fig 2: Block Diagram Hardware and Software Description

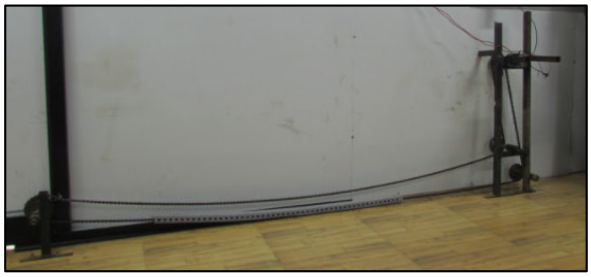


Fig 3 – Metallic Frame

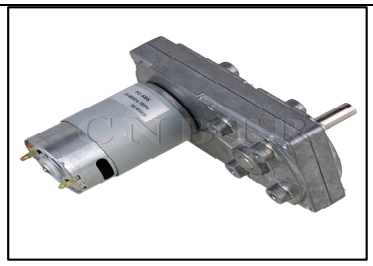


Fig 4– DC Motor

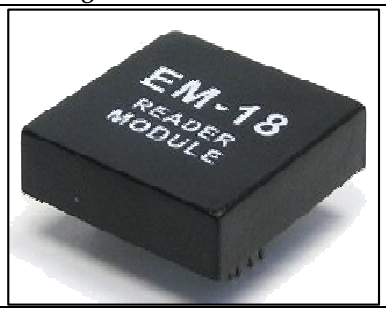
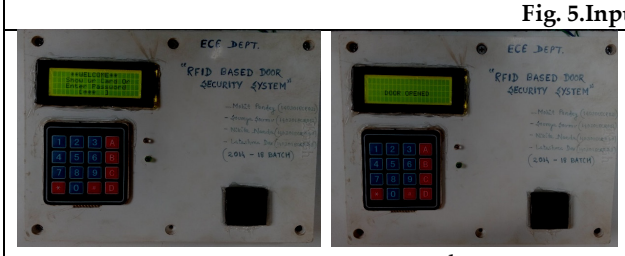


Fig 5: EM-18 RFID Reader and Tags

Fig. 5.Input Panel



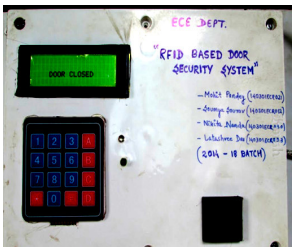
a b

Fig 6:a) Entered correct Password, b) Displayed Door Opened

a b

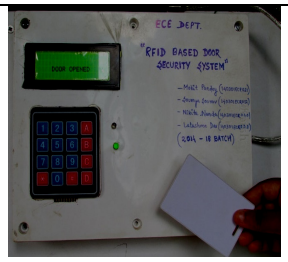
Fig 7:a) Entered Wrong Password, b) Displayed the Wrong- Enter Again

a



b

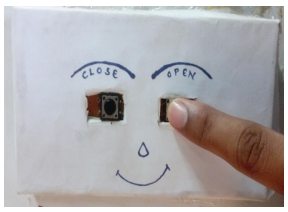
Fig 11:a) Entered Password, b) Displayed Door Closed

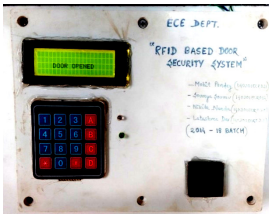


a

b

Fig 12:a) showed the valid tag, b) showed Invalid Tag





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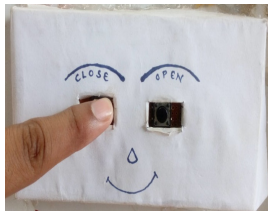

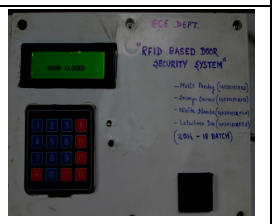

b

Fig 13: a) LCD message when the Open switch is pressed, (b) LCD message when the close switch is pressed

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RESEARCH ARTICLE

LPG Leakage Detection and Automated Booking System using LPC2129

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ABSTRACT

The rapidly developing technology has influenced human life significantly. Employing this technology to make our life easier and safer is the focus of this article. We use LPG cylinders in our homes to cook. It's quite a hazardous item in our house. It is highly flammable when it comes in contact with naked fire, even it may explode if ignored at the initial stages of leakages. So to make it safe to use safety measures are to be taken. Not all follow the safety measures even in many cases it's observed that they are ignored. Even in some cases, it has been observed that the users don't even know about the safety breaches. At this point, this prototype model comes into play. This article proposes a system that has another facility of booking the additional gas cylinder by itself, the user doesn't need to worry about running out of gas. The system uses the load cell and LPG sensor (MQ-2) as the sensing elements, it employs the GSM and LCD modules to share the information and alerts with consumers as well as the respective safety service departments. The system with help from the sensors detects the leakages and takes emergency preventive measures and intimates the same to consumer and safety service departments. Using LPC2129 is ideal because of its rugged performance, fast response, and low power consumption. The system can be further upgraded to enable the IoT feature in future applications.

Keywords: LPC2129, LPG, MQ-2, Load Cell, GSM.

INTRODUCTION

Using LPG casually and carelessly may cause a fatal result. So safety is the priority of this article. Many accidents minor or major happen daily due to carelessness and ignorance. This proposed system would help consumers to continuously monitor and remind of the safety procedures. It also takes the responsibility of the consumer's comfort by booking a cylinder for well before it runs out of gas. The system has the following components connected to it to help the consumer safety as shown in figure 1. The sensors would feed the detected information to the processor and

it would perform some calculations, comparisons and then take necessary steps as suits and mentioned the internal program code.

LPC2129 is a modern processor of the ARM7 family. It is interfaced with components like:

1. Load Cell to monitor the available weight of the gas cylinder
2. LPG Sensor (MQ-2) to detect the PPM of gas found in the surrounding atmosphere
3. Buzzer to alert the consumer of any anomaly detection
4. LCD to display the anomaly and information
5. GSM module to communicate with the safety service Departments and the consumer when needed.
6. DC motor with a driver that is used to automate the operation of the gas regulator.
7. Relay module to operate the exhaust fan as needed.

Related work

Quite aseveral systems have been proposed in the near past to make the use of LPG safe and convenient. The systems used to detect the level of LPG in the closed area of the kitchen and takes necessary actions to alert the consumer [1]. If the content of LPG in the air is significant i.e. more than 1.8% or higher it becomes quite explosive. Few authors have proposed the use of NodeMCU to detect and intimate the consumer over the android platform [2]. Automatic detection of LPG is quite a process preferred by the researchers to help the prevention of accidents caused by LPG [3]. Booking of LPG gas has become quite a simple job due to the interactive IVRS system used by the suppliers [4]. But it is not that helpful for peoples in rural areas and old age people living away from their young ones. A detection system using Arduino UNO R3 and MQ-6 is also proposed to aid the similar purpose of this article [5, 6].

PROPOSED METHODOLOGY

Many discrete components installed and interfaced together make a system functional system. This system under consideration has the following components:

Load Cell: It works on the principle of Wheatstone bridge. These have a piezoelectric strip adhered to an aluminum block that supports the weight under consideration. This weight would introduce small stress which gets transferred to the piezo strip and the resistivity changes making the bridge unbalanced. Calculating the degree of imbalance, the weight is calculated shown in fig-2(a)

MQ-2: This is a sensor that has a chemically active material inside it. The concentration of LPG changes its electrical property which is then interpreted to equivalent data and communicated to the processor shown in fig-2(b).

Buzzer: It is a piezoelectric material that is capable of generating high-frequency acoustic sound when DC supply is applied.

LCD: It's a monochromatic display, capable of displaying 20 characters each in 2 rows.
GSM Module: It's a communication module capable of making communication equivalent to a mobile phone fig 2(c).

DC Motor: It's a motor that is used in an arrangement to control the regulator electrically through a controller.

Relay Module: This component makes it possible to control high voltage appliances through controller working on small voltages.

RESULT AND DISCUSSION

The system on start-up initializes the program and checks on the sensors. First, it checks the weight of the LPG left, if it's more than the minimum, then the system is programmed to execute the next segment as in fig 4(a). Else the system initiates the LPG booking procedure and sends an SMS with the consumer number and address to local authorized LPG distributor and the consumer as in figure 4(b) and 4(c).

Secondly, it checks the MQ-2 for LPG detection. If no leakage is detected then the system goes back to the normal operation shown in fig 5(a). But if any leakage is detected (Fig 5(b) then immediately the regulator is turned OFF through the DC motor arrangement and exhaust fan is turned ON as shown in fig 5(c) and 5(d). The message communicated to the consumer is shown in fig 5(e). If leakage persists after the preventive measures then a message bearing the information of the LPG consumer number and location is sent to the corresponding safety service departments as shown in fig 6(a) and 6(b).

CONCLUSION

This system proposed is a versatile system that is fast, rugged, and flexible to upgrade. The sensors used can be replaced by industrial or commercial sensors depending on the place of application. Since it is flexible to upgrade, IoT and ML,etc can be implemented to make the system autonomous, more interactive, and intelligent.

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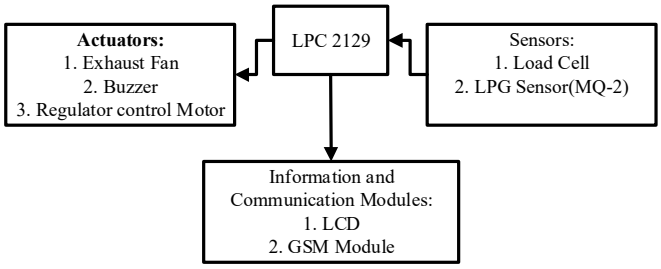

Fig 1: Proposed System Block Diagram

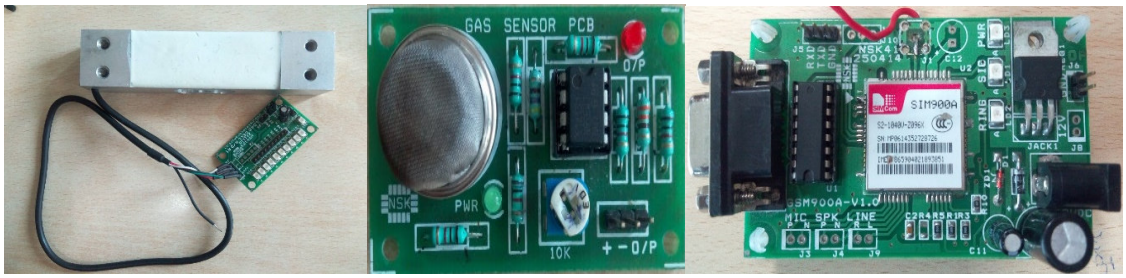

Figure 2(a): Load Cell **Figure 2(b): MQ-2** **Figure 2(c): GSM Module**

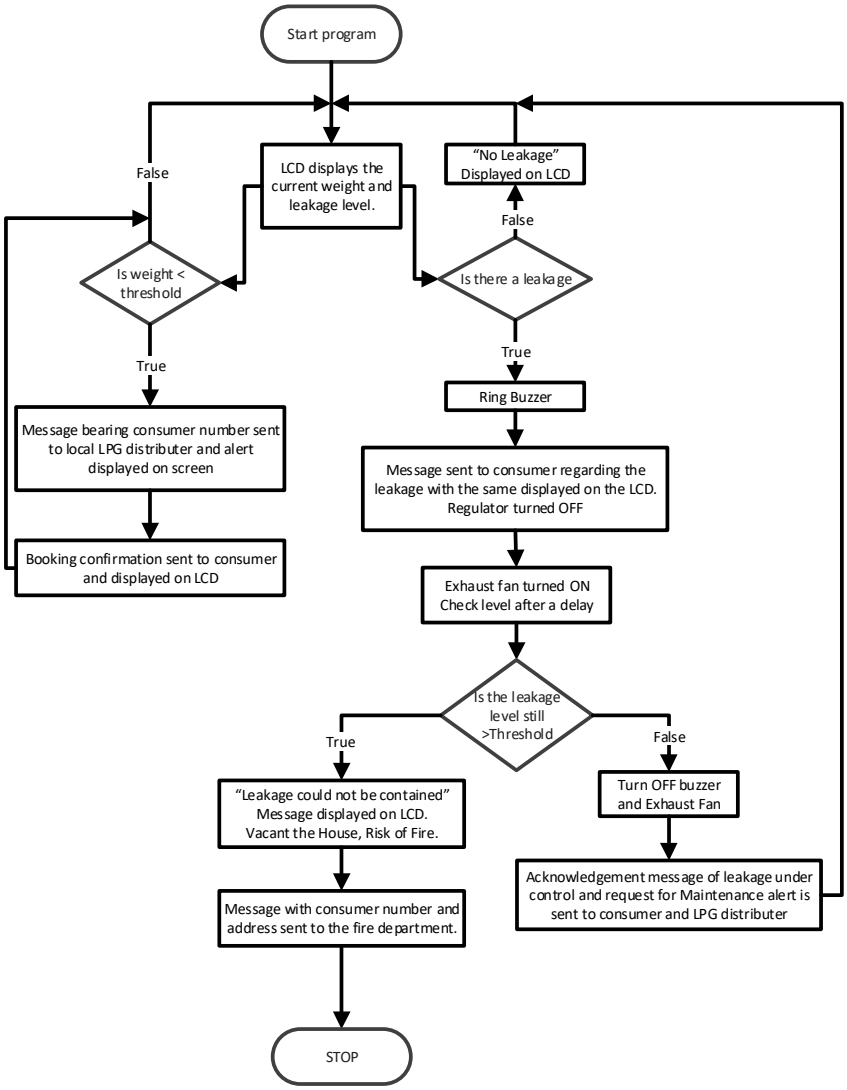

Figure 3: Proposed System Flow Chart

Fig 4(a): Load Cell Reading.

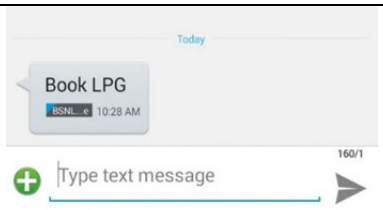

Fig 4(b): LPG Booking Information

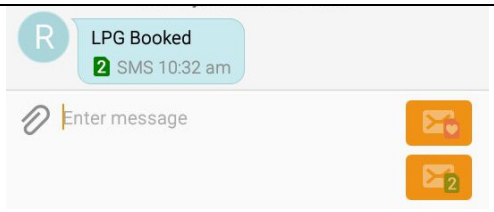

Fig 4(c): Booking Status Message

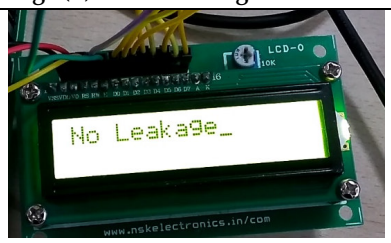

Fig 5(a): No Leakage Message

Fig 5(b): Leakage detection message

Figure 5(c): Regulator turned OFF

Figure 5(d): Exhaust fan Turned ON

Figure 5(e): Message to Consumer Regarding Status of LPG.

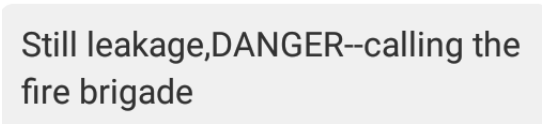

Fig 6(a): Leakage persisting message

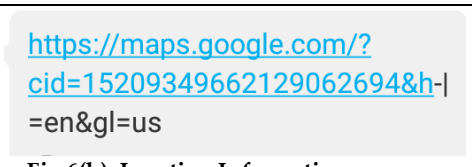

Fig 6(b): Location Information message

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RESEARCH ARTICLE

Remote Monitoring Controlling and Automation of Protected Environment Cultivation

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ABSTRACT

In this era of 21st century, there is a vast enhancement in the technological sphere, different tools and techniques are available for the betterment of the agricultural sector. To maximize the agricultural outcome and to reduce human interferences, there is a need to switch to new technology named the Internet of Things (IoT). IoT is a network of devices to transfer information without human intervention. Hence, to obtain high productivity, IOT works in association with agriculture to obtain smarter methods of farming. Coming to IoT, it deals with sensors and actuators, just like human beings have sense organs to sense some changing characteristics and react to them according to the instructions given by the brain. Similarly, IoT is all about sensing a changing characteristic through sensors (highly sensitive) and sending the obtained changing data to a processor.

The processor actuates the actuator (action) according to the requirements. This is how a system is designed (Embedded Systems). All the data that a system receives and sends are stored in a database (back-end) and accordingly is updated on the webpage (front-end) which is, later on, made accessible to the user through a website. These top technologies can add the next step to the traditional method of agriculture adding a better way of production. Sensors like soil moisture, DHT-22 (Temperature and Humidity), gas sensors are used for sensing different important parameters for crop growth (like water, sunlight, carbon dioxide, temperature, moisture). These data received by the sensor are sent to a processor (Raspberry pi 3 B) that is, the decision making unit to take the required action and hence, actuators like motor (water irrigation), solenoid valve (irrigation), UV LED's (light intensity), bubbler (moisture) start their actuation properties in accordance to the signal given by the processor.

Keywords: IoT, Embedded Systems, Automation, DHT-22, LDR, Soil Moisture sensor, Green House, Database, Webpage, Gas sensor, Raspberry pi 3 B.

INTRODUCTION

Traditional agriculture includes human intervention and the resources provided to the crop were as per human decision as the plants were not able to convey their needs. Today, in the rising era of technology things (Living/Non-living) are made intelligent enough to convey their needs and this is where the IoT (Internet of Things) comes into the picture. Every object has several unique identifiers, which makes them different from others. The technology uses this unique identifier as a base of communication. Specific UIDs have characteristics change when there is a change in the surrounding. Sensors are the objects that are highly sensitive to any change.

They are triggered with a small power but can actuate devices consuming more power, sensors can determine this change in UIDs, for example, the unique identifier of soil is the moisture content in the soil if the moisture content is less or more a signal will be sent to actuating devices(solenoid valve) to provide the soil with water now in between the sensors and the actuators lies a decision-making device which will process the signal provided by the sensor to it and accordingly the actuators have to react, parameters like temperature and humidity as its UIDs of the atmosphere and this rise or fall in temperature or temperature are detected by the sensor (DHT22) which can sense this fluctuation in the Environment and trigger the actuating devices(fan/bubbler) to maintain the atmospheric balance.UID of water is level of water which in turn can be perceived by sensors (float sensors) which after perception can cause a device to function(sump motor) alike the same concept UID of light is the intensity at it is sensed (LDR sensor) and the actuators provide the plant with light (UV led, red or blue LED), carbon dioxide concentration can also be monitored through gas sensors to monitor the carbon dioxide content in an area henceforth all the parameters that a plant requires can be monitored and controlled with sensing parameters and actuating devices thus a plant grows in a controlled environment with proper resource usage and management,Now to make the entire setup completely IOT enabled the entire operation that is perception and action has to be stored in a database and displayed in a webpage for safe storage of data for few future analysis, study and implementation.

IoT has four layers Application layer, Transport Layer, Network layer, link layer, and perception layer. The application layer is an abstraction layer that specifies the shared communications protocols and interface methods used by the hosts in a communication network, the Transport layer is a layer in the open system interconnection (OSI) model responsible for end-to-end communication over a network, it provides logical communication between application processes running on different hosts within a layered architecture, link-layer it is the lowest layer in the internet protocol Suite, the networking architecture of Internet the link layer is a group of methods and communications that only operates on a link that a host is physically connected to, the perception layer is the lowest layer of the conventional architecture of IoT, This layer's main responsibility is to collect useful information /data from things or Environment(such as WSN, heterogeneous devices, sensor type real-world objects, etc.).

The rest of the paper comprises of section II presents the Literature Survey, controlling the climatic conditions of the crop field is covered in section III, controlling the irrigation is covered in section IV, the system design along with the block diagram is explained in section V, the hardware and software components used are explained in section VI, we further described the IoT-Web integration in section VII, Section VIII covers the Implementation & Results, finally, the paper concludes in section IX with Future Works and its applications.

LITERATURE REVIEW

IoT is a growing field in technology over the past two decades and emerging to be the first preference when it comes to making anything intelligent like a complete human being is made of several systems (digestive, nervous). IoT is such a system where it can send and receive data through widespread network either with wired or wireless communication. Machine learning can only be implemented if at all there is a system that sends, receives, and stores data over a network so IoT is the foundation stone for new solid and emerging technologies like Machine learning [1]. IoT in agriculture is a benchmark and paves a path towards good productivity, high yield, proper resource

management, and more likely here crops speak, and accordingly, actions are taken [2][5]. Some of the top challenges that agricultural sector face is making the atmosphere suitable enough for plants, improper irrigation, proper nutrition to the plants, disease management, and all these problems can be solved only when the problems are detected by the crops growing in the field (it's just like a patient can describe his/her disease more appropriately to a doctor than anybody else) only then the problem is solved when it is detected that moreover saves resources [3][4]. IoT enabled systems has a strong grip on perception (sensors), actuation, storage (for further analysis) and linkage this overall package makes it more suitable for agricultural automation and preventing human intervention in agriculture thus the growing global population would reach 9.6 billion by 2050 and to provide food to this mass agriculture needs to embrace IoT [7].

PROPOSED METHODOLOGY

Overall this system shown in figure 2 is divided into four parts. i.e. Actuation, Controlling, Sensing, and Data Base Management. We have also designed the web page so that we can see the output shown in figure 5.

Controlling

We have used Raspberry Pi 3B for controlling. It is consisting of 40 pins, each pin has specific GPIO pin and different functionality.

Sensing

We have used different both analog and digital sensors. Analog sensors are soil moisture sensors and MQ2, as we cannot interface analog sensors with the raspberry pi directly so we have used MCP3008 which is an ADC. Soil Moisture Sensor used to sense the Moisture tension inside the soil whereas MQ2 helps to measure the CO2 level inside the glasshouse. Digital sensors are float level sensors and DHT22. Float level sensor used the know about the water level using the buoyance principle. DHT22 is used to measure the temperature and humidity inside the glasshouse. Sensors give the Data to the raspberry pi.

Actuators

Here we have used five Actuators used i.e. LED, sump, Bubbler, Fan, Solenoid valve. We have made the led using the combination of UV, Blue, and Red led to replacing the sunlight for the growth of the plant. Sump motor helps to lift the water from Bucket to overhead tank. When the humidity is a high fan will be on to control the humidity and temperature. Solenoid valve used to control the flow of water from the overhead tank to soil bed.

Database Management

This is used to take the data from the raspberry pi and store it in the database. Here we have used PHP and MySQL for creating the database and storing the data from the raspberry pi to the database. We have designed the web page using HTML and CSS and connected the database with the web page using PHP shown in figure 4.

We have designed the glasshouse having three soil beds, bubbler, and overhead tank. The soil bed is having 40% soil, 40% vermicompost, and 20% sand in it. Inside the overhead tank and bubble tank, we have fixed a four-level sensor to know about the status of the water level. Inside the bucket, we have a fixed sump motor. Water from the sump motor goes to an overhead tank if both the status of the float sensor is low. Then the water from the overhead tank goes to the Soil bed and Bubbler according to the status of the soil moisture sensor and the status of the float sensor present inside the bubbler.

Monitoring & Controlling Climatic Conduction of Green House

The parameters that are to be controlled for the crop are temperature, humidity, and the amount of carbon dioxide content in the atmosphere. The sensor that determines as well as perceives the humidity and temperature is DHT22 which has an NTC (negative temperature sensing Coefficient) and a thermistor (a variable resistor that changes its

resistance when temperature changes.). These variations in resistance are interpreted and recorded through a processer (Raspberry Pi) by a certain programming methodology.The processor is programmed as per to react which change in variation for example if the temperature exceeds 30 degree Celsius the fan has to be in ON state automatically until the temperature drops to certain level same goes for humidity sensing factor, in between two electrodes lies a substrate that changes the conductivity of the electrodes after humidity perception and thus a bubbler (provides additional humidity if required)reacts at one of these varying conductivity of the electrodes as per processing unit in concern to the programming logic that is implemented.The light intensity is handled by LDR (light dependent resistor).It is a component whose resistivity changes when light intensity increases or decreases adding to this variability the UV LEDs, red LED's and blue LEDs (lights required for crop growth) are set ON or OFF as per need.

Monitoring & controlling Crop Fields

The moisture property of the soil has to be maintained through the right stimuli and that is achieved by a soil moisture sensor. The moisture sensor uses capacitance property to measure the dielectric permittivity of an area. This sensor averages the water quantities in the soil. Now this changing property (Dielectric Permittivity) acts as a stimulus to the processor via programming methodologies. Accordingly, the irrigation system that is set up is available for the soil that is, the solenoid valves placed in the pipelines are opened in case the water content is less which signifies that both water content for the plant and soil needs to be maintained. This entire process is very vital for irrigation purposes as the actuation depends on the property of the soil to hold moisture. This is how the soil is directly speaking to the processor to make the water available for it and the processor is reacting to the stimulus received from the soil by opening the solenoid valve.

Availability of water: The entire irrigation process depends on the availability of water. To check the availability of water we need to consider a parameter that is, water level. To sense the level of water we use float sensors, which are setup inside the overhead tank or the water storage house, one at the top and one at the bottom. The float sensor acts as a switch. When the level of water rises and reaches the brim, the sensor reads high voltage and signals the processor which in turn is connected to the sensor to terminate the motor as the overhead tank is full. The float sensor at the bottom indicates that the overhead tank is empty as it reads low voltage and signals the processor to switch ON the motor, to, make the water available to the soil refer figure 3.

IoT Web Integration

Web integration with IoT enables people with all information they demand. IoT is a straightforward concept that has to be related to the web to be accessed, configured, and manipulated correctly with the associated sources (mobiles, smart devices, etc.). To establish this connectivity IoT is integrated with web design. Web designing is more complex as a designer has to think of front-end and back-end design. The webpage is created using HTML, CSS, and JavaScript in-order to represent the data at the front-end. Front-end is created to communicate with users through smart devices. At the back-end, the database has been created using the tool, phpMyAdmin, to fetch the data from the sensors via processor using PHP scripting language and accordingly update it through a certain interval. A reference table is present along with the current data table for comparing the data and accordingly, the actuation takes place. Actuation happens depending on the required conditions for a certain type of plant.

Hardware and Software Description

Hardware used

The Proposed System consists of hardware like a Raspberry Pi Model 3B, Float level Sensor, DHT22, Soil Moisture Sensor, Bubbler, MQ2, MCP3008(ADC), Solenoid Valve, relay Module, and SMPS 450 Watt.DHT22 sensor is known as the Temperature and Humidity sensor which is used to give the exact temperature and humidity value to the processor for further actuation. MCP3008 which acts as a 10-bit analog to digital converter. Generally, in a Raspberry pi, all the pins are digital pins, so to interface analog sensors to the raspberry pi we have used this IC which acts as a

converter, converting an analog value to digital. The gas sensor is used to sense the carbon dioxide content present inside the greenhouse. We are considering the analog output from the gas sensor and providing it to the MCP3008 to get the digital values. We have made the led setup using red, blue and UV led for proper growth of the plant. Float Level Sensor is used to know the level of water inside the tank using the buoyance principle.

Software used

The system is incorporated with the following software for the functioning of the whole system. There are Raspbian operating system which supports Python, phpMyAdmin Database, Apache Server, MySQL. Steps to install the Raspbian OS

1. Download NOOBS and extract it
2. Format the SD card
3. Put the Noobs Files on the SD cards
4. Put the SD card into the raspberry pi and
5. Power up the raspberry pi for booting of OS.
6. Upgrade and update the OS.

Steps to install the Apache Server

1. Use the command in the terminal sudo apt-get install apache2.
2. Check for Apache is working properly or not by using any web browser.

Steps to install PHP

1. Install suing command Sudo apt-get install libapache2-mod-php7.3 php7.3

Steps to install the phpMyAdmin,

1. Type command sudo apt-get install php php-mbstring
2. Use command sudo apt-get install phpmyadmin
3. Add "Include /etc/phpmyadmin/apache.conf" in path /etc/apache2/apache2.conf
4. Start the connection suing /etc/init.d/apache2 restart
5. Check phpmyadmin is working or not by open any browser and typing http://localhost//phpmyadmin
6. Give the user name and password

Steps to install the MySQL

1. Use of command on the terminal sudo apt-get install mariadb-server-10.0
2. sudo apt-get install php7.3-mysql
3. Verify MySQL is working properly or not

Step to install dht22 library

1. Enter the below command to download the library.
   git clone https://github.com/adafruit/Adafruit_Python_DHT.git
2. Then enter into the installed directory using the below command.
   cd Adafruit_Python_DHT
3. Now download the required modules using the below command.
   sudo apt-get install build-essential python-dev
4. Then install the library using the below command.
   sudo python setup.py install

Step to install spidev for Soil Moisture

1. Start by launching the terminal and typing in the below command:
   sudo raspi-config

2. Navigate to the interfacing options.
3. Enable the SPI interface.
4. Reboot your Raspberry Pi.
5. Now install spidev library.
6. sudo apt-get install git python-dev
7. git clone git://github.com/doceme/py-spidev
8. Go inside the directory cd py-spidev/
9. sudo python setup.py install
10. install numpy library
11. sudo apt-get install python-numpy

PhpMyAdmin is a free software tool written in PHP and can handle the admiration of MySQL over the internet. MySQL connector is the module present in the python for inserting the database into PhpMyAdmin internally. We have also used the HTML, CSS for designing the web page. PHP also used for connecting the python code with the web page and database with the web page.

Simulation Results

The proposed system is divided into four-part: 1) Sensing, 2) Actuation, 3)Controlling, 4)Data Base Management. Firstly, coming to the sensing parts, we have used both analog and digital sensor i.e. DHT22, Float level Sensor, Soil Moisture Sensor, MQ2. We have used Raspberry Pi for the controlling process. Sensors give the data to the controlling and according to it, actuators do its respective work. Actuators used are led, Solenoid valve, Bubbler, Fan, Sump Motor. Lastly, coming to the database management raspberry pi take the data from the sensor gives to the database and then the results are store in the database every second and then displayed on the web page shown in figure 4. We have used PHP, MySQL, HTML and CSS shown in figure 5. Refer figure 6 and 7 for more details.

Case1. First of all, we have used a sump motor inside the bucket so that we can lift water to the overhead tank and inside the bucket, we have fixed one float level so that whenever the water level goes down the pump motor will be off and the whole system will stop working.

Case2: We have designed over the header tank so the water from the sump will go to the overhead tank than from the overhead tank from will go to the soil through the drip irrigation method by the operation of the solenoid valve.

Case3: We have fixed the soil moisture sensor in all the soil beds so that if the soil tension inside the soil bed increases then the solenoid valve will be on.

Case4: Inside the overhead tank we have fixed two float level sensors so that if both the float level sensor gets high condition then the sump will be off and both get low condition then the sump will be on and the same in the bubbler.

Case5: Water from the overhead tank goes into bubbler and also inside bubbler we have fixed two float level sensors so that if both are low then the solenoid valve will open and water from the overhead tank will go into the bubbler.

Case6: We have fixed dht22 for measuring the temperature and humidity sensor so that if the humidity is low then bubbler will be on and if the temperature is high then the fan will be on.

Case7: We have used the combination of UV, blue, and red led in replacement of sunlight of the growth of the plant. Here we have set the time from 5.00 am to 6.00 pm the led will be on otherwise it will be off.

CONCLUSION

We know to feed this vast population there has to be a change in the way agriculture is carried out and this change is IOT implementation in agriculture. Human beings are efficient because they can sense, process, act themselves and don't need any intervention and the same has been done to crops inside a greenhouse the are provided with a controlled and protected environment where they can sense their needs via sensors, processor and actuator which makes them more efficient furthermore like a human if a machine could take its own decision (machine learning) that will be a revolution to agriculture. Agriculture should be availed with a wide range of scopes like disease

detection which is very vital because plant should be healthy to be fruitful which can be done through a pi camera and we can even monitor the plant's growth hence this entire process will be a system which can detect its disease and need and act accordingly which will be the next step to agriculture development with technology in hand.

ACKNOWLEDGMENT

I would like to acknowledge my friends involved who have accompanied me in completing the work and I would like to pay my sincere regards to my faculties, who have guided and mentored the entire process of the project has a great impact on agriculture and I pay my gratitude towards our University for rendering all support needed

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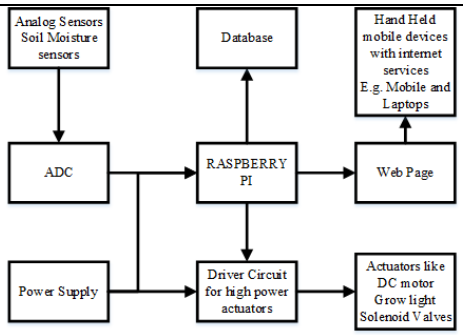


Fig 1: Block Diagram of Green House

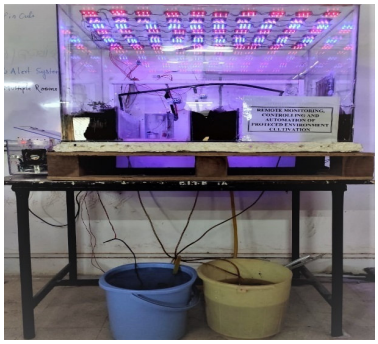


Fig 2: Proposed System

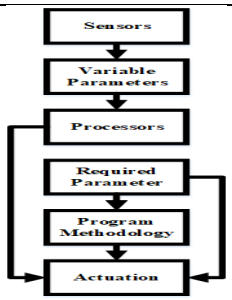


Fig 3:Entire Data Cycle

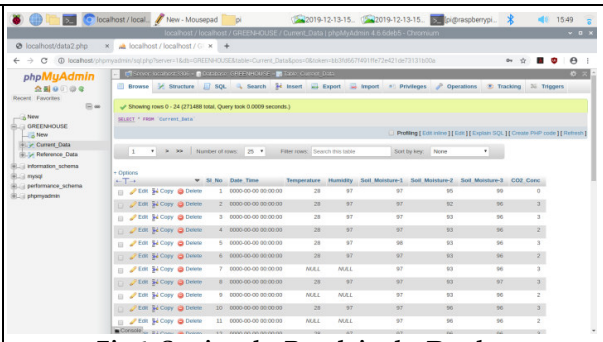


Fig 4. Storing the Result in the Database

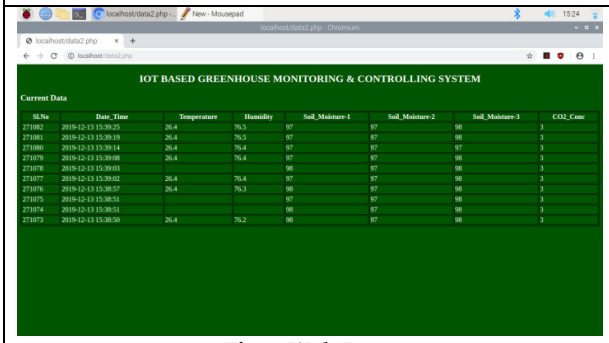


Fig 5. Web Page

Fig. 6a

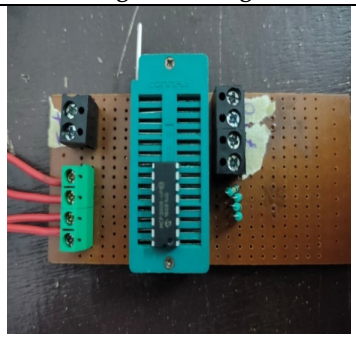


Fig. 6b

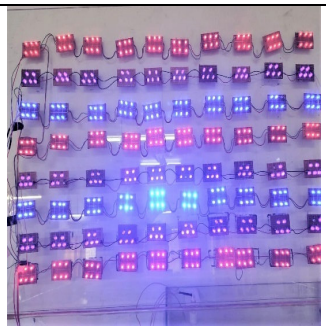
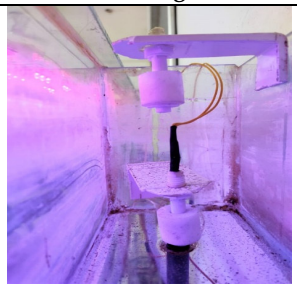


Fig.6c

Fig 6 (a) Soil Moisture Sensor(b) MCP3008, (c)LED Lights



a

b

Fig 7.(a) Float Level Sensor (b)Soil Bed with Solenoid Valve.

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RESEARCH ARTICLE

ARM 7-Based Alcohol Detection and Accident Prevention of Vehicle

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ABSTRACT

The main purpose of this project is the identification and detection of "Drunk Driving". Nowadays, if observed it will be quite clear that drivers after getting drunk face accidents on road. So drunk and driving is a major reason for accidents in almost all countries all over the world. This article is concentrated on the designing of an alcohol detection system to be installed inside the car for the safety of the passangers and the driver himself. The accident prevention system is a flexible system that detects the alcoholic level of the driver and takes steps accordingly. The use of LPC2148 microprocessor to implement this project is selected due to its rugged and low power consumption, its quite reliable and stable during operation. The MQ-3 sensor is used to detect the percentage of alcohol in human breath when exhaled on to it. Alcohol sensors give out analog data that can be analyzed by the LPC2148 microcontroller. The data received from an alcohol sensor is converted into digital form with the help of a digital converter (analog to digital convertor), after that the data is stored in microcontroller and then compared to the threshold values. If the value is beyond its set limits, then with the help of the program controller takes appropriate action which controls the ignition system. Here we used relays to control the ignition system. In this project by controlling the ignition system, we can prevent the accident that occurs due to drink and drive.

Keywords: LPC2148, GSM Modem, GPS Module, Alcohol Sensor,DC Motor

INTRODUCTION

Drink and Drive is the cause of most accidents observed all over the world. An Alcohol Detection system istalled inside in the vehicle would be quite convenient to track the driver's condition continuously to ensure the safety of the passangers as well as the driver himself. This project is designed to be installed inside the car and maintain a

continuous monitoring system inside it, the system is also facilitated with communication system that conveys information to the base station or the concerned person regarding the current status inside the car related to Alcoholism. This system used a GSM and GPS module to to track the vhicle and parallely the processor takes necessary preventive measures to avoid accidents as much possible. This can also be utilised for vehicle tracking in case the vehicle is stolen.

The modern smart phones are loaded with various physiological sensors with advanced communication capabilities powered by high speed internet capabilities. So the sensors in the smart phone can be utilised to detect a number of parameters to monitor in the project. Using the Bluetooth and Wi-Fi communication system the sensors in the smart phone is utilised for the project. The project would clarify the basic idea behind the tracking algorithm developed in this research. For individual vehicle tracking the first step, acquisition image sequences, and predetermining the detection zones at each lane. Second, we have conducted background subtraction.

Drinking and driving is already a serious public health problem. Its is a severely affecting the public as the number of accidents is increasing significantly due to the consumption of alcohol. This article presents the use of alcohol detector,a device that senses a change in the alcoholic gas content of the surrounding air this device is more commonly referred to as breath analysis, as it analysis the alcohol content from a person's breath. The system detects the presence of alcohol in the vehicle and slowly takes controlof the vehicle as well as establishing a continuous communication with the base station.

LITERATURE SURVEY

The background study for a project is necessary. This enables the tracking progress of the project effectively. In a system it is proposed that by analysing the the video and images of the driver it can be determind that how much attention the driver is having on the road. It uses the analysis of facial orientation, appearance of eyes, position of eyes etc. Another proposed system deals with implementation of AI that analyses the drowsiness and fatigue of the driver. The moment the system finds any anomaly it takes over. Using image analysis the contour of mouth while yawing is also detected to estimate the drowsiness of the driver. System with AI and Neural network based algorithms are used to analysis the drowsiness through video analysis. It warns the driver and lets information passed on to the next level.

PROPOSED METHODOLOGY

The whole system is divided into three parts, they are 1) Input device, 2) Output devices, 3)Controlling Unit. The devices which are input to the system are Alcohol sensor , GPS, GSM. Wheras the output devices are the mobile phones, the LCD display. The main controlling unit here is the LPC2148 ARM 7 Processor based controller. All the input and output device are interfaced to the main processing unit by wired and wireless medium. The input devices are acting as a sensors , which sens the physical parameter in analog form and send it to the controlling unit. As we know that in Embedded System, controlling devices like microprocessor and microcontroller can only understand the digital signals. So wen the input devices send any analog signal we have to convert the signals into the digital by using the ADC. ADC play an very important role. The main function of ADC is to convert the analog signal received from a sensor into the digital form. The ARM controller used here has the inbuilt ADC functionality, with a 10 bit resolution. Hence external interfacing of ADC is not required to the microcontroller unit. Once the alcohol sensor senses the percentage of consumption in the form of analog value it send to the microcontroller unit . The microcontroller directly sends it to the ADC unit , which then convert it into the corresponding digital values.

Next part is the GPS traker , it's a satellite based system which drives independentely.It is directly connect to the main controlling unit using only 2 pins names as TXD and RXD. GPS has the capabilities to track the position in the form of Longitude, Latitude, with Date and Time. There are different version and types(size) of the GPS module

available in the market. It receives the location from the satellite for every second. It works using the NMEA protocols This information can be view in the serial monitor of the IDE used after programming. The NEMA protocol consists of 19 Interpreted sentences which starts with $GPxxx. This advantages of GPS makes it widely used in many applications like tracking and surveillance. This is much more accurate to about 14 ns.

The last important part in this prototype model is the GSM module. This module available in market in many size and shape with variable price like SIM900, SIM700, SIM800, SIM808 etc. Before interfacing one has to choose the appropriate module which suits the application. This module is interface to any microcontroller with the help of UART protocols. It helps in sending receiving data over GPRS, send and receive SMS, make and receive voice calls. To activate any fuctin listed above one has follows some AT commands. AT commands is used to configure the system to perform like a call and SMS. The power input to this module is 12 V, 2A. It has built in LED to show power on and off, network leds. When modem is powerd up the network led starts blinking and when the network registration is over , it starts to blink every 3sec. Testing can be done in serial monitor by using the 'AT' command which return back 'OK'.

So the model is equipped with a smart technologies, now if a driver is totally drunken then the System will never start.Through programming the system threshold value for the percentage of the alcohol consumed is set. The proposed flow diagram shown in figure 2 describes the working of the whole system. After the power is turn on all the devices goes to the active state. The Alcohol sensor is continuously sensing the alcohol is consumed or not by the driver. If the driver has not consumed the alcohol then the vehoicle will run smoothely. There is no disturbanvce from the end of the smart sensors implanted inside the vehicle. The system is designed in such a way that, if the percentage of alcohol consumed is less than 30 % than the vehicle engine gets on and it work in normal mode. If in case the percentage of the alcohol consumption is more than the threshold value then the ignition never starts and its send an imformation to the relative of the driver. By using the GPS module and GSM module installed inside the vehicle. GPS module detects the exact location of a vehicle with Longitude and Latitude. Whereas GSM module will send information about the longitude and Latitude to relatives of the driver.

Simulation Results

The below algorithm gives an idea of how the setup works for a single run of the code.
Step1: Include all Header files.
Step2: Declare different functions used and global variables.
Step3: Define delay functions and LCD related functions are being declared.
Step4: UART function was defined
Step5: ADC function was defined.
Step6: Then Alcohol sensor related functions are being declared.
Step7: Main function is started and different variables used in the program are declared.
Step8: Both the codes of GSM+GPS have been merge together and their function declared
Step9: PWM function was defined
Step10: last step is to compile , debug and create the hex file.
Step11: when the hexadecimal file is created using the IDE, it has to be uploaded using the flash magic to the target hardware.

The fig.3represents the interface between GSM SIM 800A Module with LPC2148 Microcontroller. Here we have connected the RX and TX pin of GSM to P0.0 and P0.1 of LPC2148 respectively. Here we have successfully sending the message via GSM through microcontroller as per figure 4.After that we have received the messages shown in figure 5(a). When the alcohol consumption ratio is less than 20%,the motor will rotate in its normal speed (duty cycle 100%) shown in figure 6(a).When the alcohol consumption ratio is greater than 20% and less than 40% the speed of the motor will be reduced (duty cycle 50%) shown in figure 6(b).

When the alcohol consumption ratio is greater than 40%, the speed of the motor comes to halt (duty cycle 0%) shown in figure 6(c). The vehicle stop functioning. As soon as the motor will come to halt, a message will be sent via GSM specifying the location of that particular vehicle through GPS which is shown in figure b(b).

CONCLUSION

This proposed system is simulated and tested in lab conditions. It is observed that the system works well within the designed parameters. Usage of more powerful processors to do more heavy and complicated computation would enable implementing new techniques like machine learning that would make a study of the driver behaviour and take necessary actions. This would be more appropriate to use of the machines we use are autonomous. So that the system can takeover the human activity and take everyone in the vehicle to safety.

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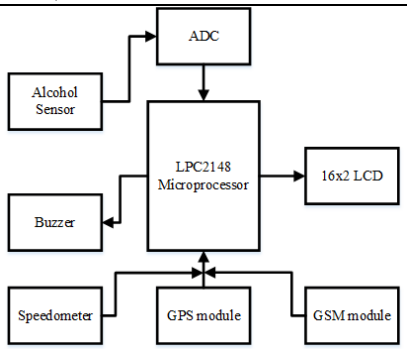


Fig1: Block Diagram of Proposed system

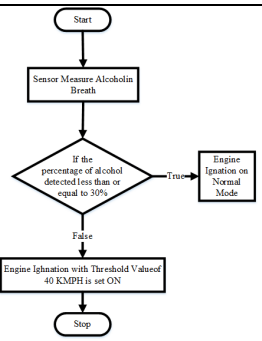
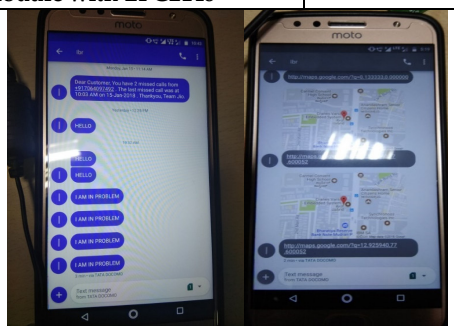


Fig 2: Proposed System Flow Chart

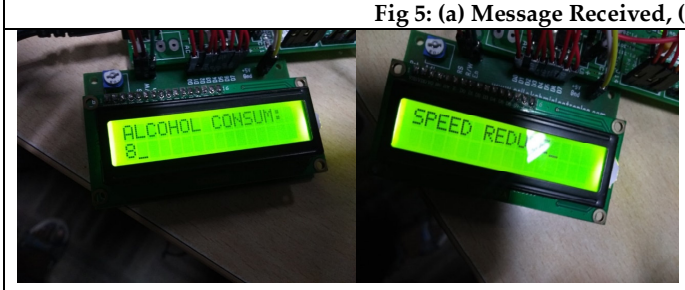
Fig 3: Interfacing of GSM module with LPC2148

Fig4: Message sent

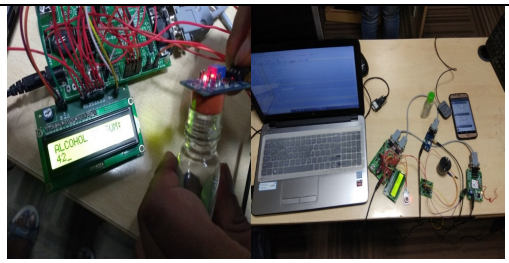


a **b**

Fig 5: (a) Message Received, (b) Live Location



a **b**



c **d**

Fig 6: (a) Alcohol consumption <20% , (b) Speed reduced , (c) Alcohol consumption <20%(d) Complete Setup

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RESEARCH ARTICLE

Design and Implementation of Dual Port SRAM

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ABSTRACT

In microprocessor the large SRAM arrays are used which occupies major portion in the die and it is extremely essential to have optimized larger arrays of memories for the smooth functioning of the chips. In this work a 6T SRAM cell is designed in cadence Virtuoso and the power dissipation of 753.9µW and write time and read time were observed to be 80 ns and 10ns respectively. Further a a dual port SRAM is designed using CMOS 180nm technology in order to achieve high speed and low power consumption. To validate the result simulation are carried out in cadence platform and both front end and back end analysis were performed.

Keywords: SRAM, Delay, Power, VLSI, SoCs

INTRODUCTION

Since the evolution of System on Chip technology, memories have become the indivisible part of any VLSI system. The Traditional RAM has been classified into SRAM and DRAM[1-3]. Memory is the ability to hold information irrespective of whether it is a computer memory or human memory. There are three stages for processing of theinformation.1. Encoding: Receiving the appropriate information/data, 2. Storing: Holding the received information/writing the data3. Retrieving: Reading the data.

Computers store programs/data in the form of bits, and each bit is stored in a cell commonly called “memory cell”. A memory cell is the basic unit of a large storage device. The memory cells are categorized among volatile and non volatile memory. Various research groups around the globe are working on emerging technologies like PCRAM, MRAM, FERAM and ReRAM [4-6]. They are considered to be the potential replacement for the traditional SRAM, DRAM, and flash memory. Phase change memory is based on the material called the phase change element. These are widely used in optical storage devices, compact disc. Though it has denser structure than MRAM but it still needs further improvement on density and endurance. Magnetic RAM has shown much potential advantage over

Phase change RAM, but its complex configuration is one of the major challenges towards its implementation in the next generation memory.

The Magneto resistive RAM and Ferroelectric RAM are poorly scalable and requires large programming current during write cycle which led high power dissipation. The popular volatile memory cells are SRAM and DRAM which are well known for its high speed and are used in cache memories. SRAM contains at least 4T which leads to higher memory density [2]. The memory density can be reduced by using DRAM, which can be designed even by using a single transistor but it needs to be refreshed periodically which increases the power consumption and added to these disadvantages both SRAM and DRAM are volatile memories. Single-port SRAM enables only one read/write operation at a time where as dual-port SRAM allows number of read/ write to happen at the given time. In this work a 6T SRAM cell is designed and discussed in the subsequent sections. Beside a Dual Port SRAM cell is designed at both Front end and Backend its design parameters are analysed.

BLOCK DIAGRAM AND STATIC MEMORY OPERATION

Fig.1shows the block diagram of dual port SRAM. The input dual port SRAM consists two address lines for PORT A and PORT B each consisting of 6-bits. Further 8-bit input data lines are present for PORT A and PORT B. Beside their write enable signals are present for PORT A and PORT B. Finally, a clock signal is present which assist in synchronizing between PORT A and PORT B. Similarly, there are two data output ports A and B. The resulting structure consists of two 64×8 dual port SRAM.

The basic SRAM cell consists of two cross-coupled inverters and two access transistors. At the gate terminal of access transistor word line is connected and to source/gate terminal bit line is connected. The work of word line is to select the cell while bit lines are used to perform read and write operations on cell. Initially the cell holds stored value on one side and its complement on the other side. Let us assume initially q holds the stored value and qbar holds the complement of the stored value. These two complementary lines are used to enhance noise rejection and speed. The 6T (Transistor) Static RAM cell is shown in Fig.4.9. Here there are two pairs of cross coupled inverters. Suppose in the pair of inverters the PMOS is replaced by resistors, as now only 4T are used to make the cell, hence the name 4T Static RAM cell. The current through these resistors can be made small by using high pull-up resistances.

There are three possible mode of operation Write Operation, Hold Operation, Read Operation The data is written to the memory cell by driving the word line and bit line high. To hold the data that is written, the Bistable inverters are disconnected from the bit line by driving the word line low. The Read Operation is initiated by precharging the bit and bit bar lines high and activating the word lines, either of the bit line discharges through the NMOS of any of the inverter creating a differential voltage between the bit and bit bar line, which can be read by the sense amplifier. The Read and Write Operation of SRAM cell is shown in the Fig.2. Following table 1 explains the performance analysis of SRAM cell

IMPLEMENTATION OF DUAL PORT SRAM IN CADENCE

Verilog Code has been implemented to obtain all the top modules in cadence platform. It follows following tools to obtain both front end and backend result

- To Run Simulation: NCLAUNCH tool is used. Using this tool with implementing the test bench code the simulation result is obtained
- To Obtain RTL: RTL compiler tool is used for obtaining the RTL schematic of the design
- Synthesis Part: This section consists of converting RTL to GDSII, floor plan, power plan, placement, routing, pre and post timing analysis

RESULTS AND DISCUSSION

a. **RTL Diagram:** The RTL of the dual port SRAM has been obtained using Encounter RTL compiler. It can be observed from the result that the RTL Contains all the modules of the SRAM
b. **Simulation Waveform of the RTL:** To validate the RTL obtained for the dual port SRAM has been simulated using RTL Compiler in cadence platform. The result validates the successful execution of the read and writes operation of dual port SRAM.
c. **Timing Analysis:** For the proposed design the timing conditions is verified and it is observed to meet the requirements. The total time delay has been found as 5.60ns
d. **Cell Report:** After compilation of RTL using RTL compiler the number of cells of each module and power is obtained. It has been found there are total 65.539 number of equivalent gates are available,
e. **Backend Design:** For backend design the RTL is converted to GDSII by using ENCOUTER tool. Here netlist is imported to obtain GDSII. In this part , floor plan, power plan, placement, routing , pre and post timing analysis is being done and the layout of Dual port SRAM is obtained and shown in the below figure 6.

CONCLUSIONS

In this work we have successfully designed a 1-bit SRAM based memory cell using cadence virtuoso and investigated the power, delay and Memory access. Further in order to read/Write more number of bits from the memory cell a Dual port SRAM is designed using Verilog hardware description language. In addition to that RTL synthesis and Layout of the chip is designed. It is found that our proposed design work as desired.

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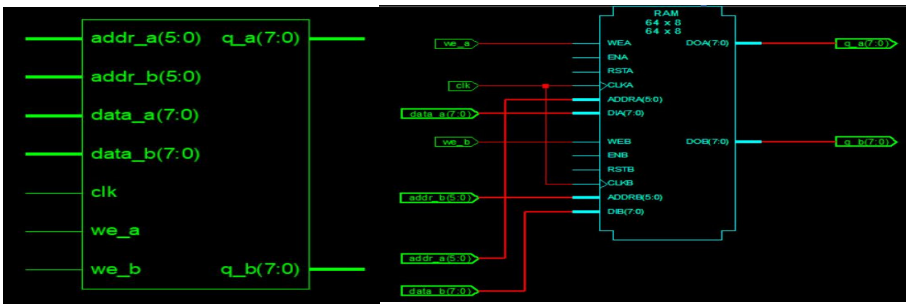

Fig.1 Block Diagram of Dual Port SRAM

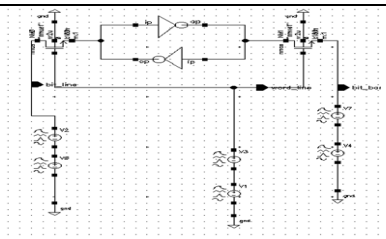

Fig.2 Schematic of SRAM

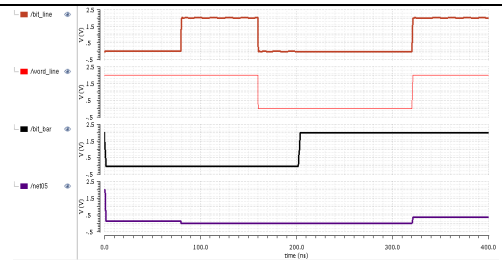

Fig.3 Read Write Operation of

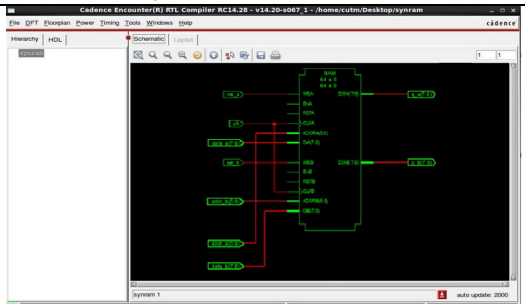

Fig.4 Top Level RTL Module of SRAM

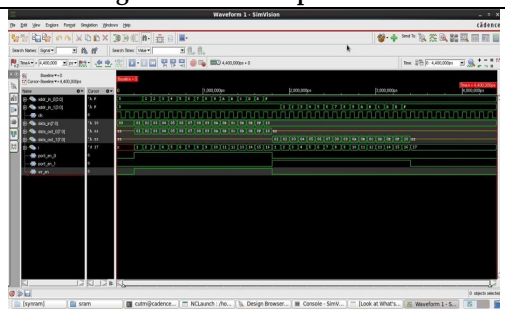

Fig.5 Test Bench Simulation Waveform of Dual Port SRAM

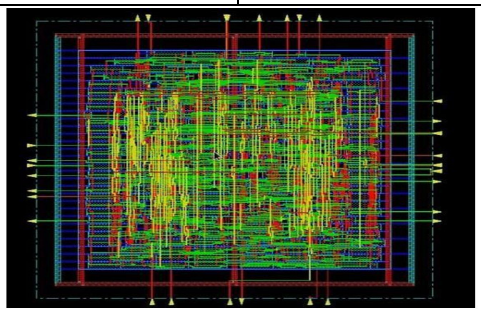

Fig.6 Layout Design of Dual Port SRAM

TABLE 1. Performance Parameter of SRAM Cell

Parameters	SRAM Cell
Power	753.9µW
Read time	10ns
Read Voltage	1.8 V
Write Voltage	1.8V
Retention time	Few seconds
Write time	80ns
Number of Transistors	6
Energy	266.7PJ

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RESEARCH ARTICLE

Design of SRAM Augmented 32 Bit Synchronous FIFO

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ABSTRACT

FIFOs are widely used for the purpose of on-chip data memories. The condition essential for the correct operation of FIFO is that the read pointer value to be sent to the write clock domain and the write pointer value to be sent to the read clock domain. FIFO memories are built using dual-port SRAM memory, where the 'Empty' and 'Full' condition of the memory is observed. In this paper a 32 bit FIFO is designed using dual port SRAM is designed which was found to be area efficient as less number of logic gates were utilized and delay was found to be considerably low as 27.136ns

Keywords: FIFO, SRAM, Synchronous, Delay, VLSI

INTRODUCTION

In all the complex digital circuits there are multiple number of circuit boards available and always exchange of data between them occurs. Hence, there is need of intermediate stages contacting memories receiving the data at the receiver end of circuit boards at high rate or in batches, but it is processed irregularly and slowly. Basically, the memories act as intermediate blocks which works at different speed. The first in first out (FIFO) memories has characteristics of the data that is entered at the first instant are getting out first from the queue. FIFO memories can be used as shift register. A FIFO memory is an electronic storage usually used between two subsystems. It has two control signals i.e. write and read. The data is written to the memory when write is enabled and data is made removed from the memory to make space for other incoming data when read is enabled. In Microcontroller peripheral the incoming data is stored using a FIFO memory asynchronously. But it cannot be read immediately. In hardware implementation the FIFO memory is used for synchronisation purposes. The FIFO memory is implemented as circular shift or queue having two pointers i.e. pointer for read and pointer for write register. To increase the bandwidth and as well as to prevent loss of data during communication the FIFO memory are used. To indicate the empty and full condition the FIFO has status flags [1-3].

When there is no dependences between reading and writing of data it's called as concurrent FIFO. In this type of FIFO both read and write operation occurs simultaneously with overlapping i.e. with different frequencies two systems are connected to FIFO memory. FIFO are basically of two types namely synchronous FIFO and asynchronous FIFO. Synchronous FIFO requires free running clock from both read and write systems. Write Enable is used to control the write operation synchronised with clock signal (write). By using the free running clock full status signal line is controlled with synchronisation with write clock [3]. The Figure 1 shows the block diagram of synchronous FIFO with its inputs and outputs

ARCHITECTURE DESIGN OF FIFO MEMORY

To overcome from the limitation of long exaction time in Long FIFOs, the a system should not shift the data words through all the memory locations. This problem is resolved by using circular memory having two pointers. Here the incoming data memory address is in write pointer. The 1st data word address in the FIFO to be read out will be in 2nd pointer i.e. read pointer. Both read and write pointers indicate to the same location of memory after reset. Write pointer points to the next memory location after the write operation. The read pointer points to the read of next data word which will be read next. Read pointer constantly follows the write pointer. The empty status of the FIFO determined when read pointer reaches write pointer. The full status of FIFO is determined if the write pointer catches the read pointer.

A dual port SRAM is used with the FIFO memory for storage. The pointer act as binary counter to generate memory address. It is better choice to have 2nd memory locations as pointer is implemented as n-bit counter. The read pointer generates read addresses and writes pointer generates address of write. The following figure shows the FIFO with dual port SRAM. It can be also designed other non-volatile memories such as RRAM [4-6].

ASIC IMPLEMENTATION OF FIFO MEMORY IN CADENCE PLATFORM

Verilog Code has been implemented to obtain all the top modules in cadence platform. It follows following tools to obtain both front end and backend result

- To Run Simulation: NCLAUNCH tool is used. Using this tool with implementing the test bench code the simulation result is obtained
- To Obtain RTL: RTL compiler tool is used for obtaining the RTL schematic of the design
- Synthesis Part: This section consists of converting RTL to GDSII, floor plan, power plan, placement, routing, pre and post timing analysis

RESULTS AND DISCUSSION

RTL Diagram: The RTL of the FIFO memory has been obtained using Encounter RTL compiler. It can be observed from the result that the RTL contains all the modules of the FIFO memory.

Figure 6 shows the top module of 32-bit FIFO Memory. From the module it can be observed that the design has 32-bit data input and output along with Read and write signal, clock, enable and reset. The output of FIFO register also indicates the two status flags for empty and full. To validate the RTL design of FIFO memory the test bench code has been generate and compiled using RTL compiler and simulated wave form is obtained in SimVision as shown in the figure 6

Timing Analysis: For the proposed design the timing conditions is verified and it is observed to meet the requirements. The delay due to gates has been found as 14.309ns and the delay due to routing wires has been found as 12.827ns. Thus, the total time delay of FIFO memory has been found as 27.136ns

Cell Report: After compilation of RTL using RTL compiler the number of cells of each module and power is obtained. It has been found there are total 4,728 number of equivalent gates are available. When implemented with Xilinx ISE it has been found there are 106 number of 4 inputs LUT among which 42 number is used as logic, 65 number used for Dual Port SRAMs, 71 number of bonded input-output blocks, and 32 number of input-output flip-flops.

Backend Design: For backend design the RTL is converted to GDSII by using ENCOUTER tool. Here netlist is imported to obtain GDSII. In this part , floor plan, power plan, placement, routing , pre and post timing analysis is being done and the layout of FIFO memory is obtained and shown in the figure 7

CONCLUSION

The FIFO memory augmented with SRAM is designed in cadence platform both in frontend and backend using CMOS 180 nm technology library in cadence. The presented work implements multiple read and write operations under the impact of single clock. From the wave forms it is observed that the proposed FIFO design was able to track empty and full flag status. Our design comprises of 4,728 logic gates and delay performance was found to be 27.13ns.

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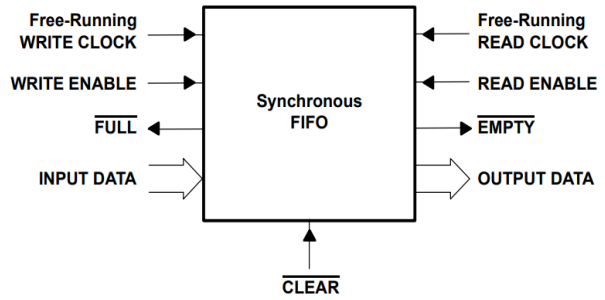

Fig.1 Block Diagram of Synchronous FIFO

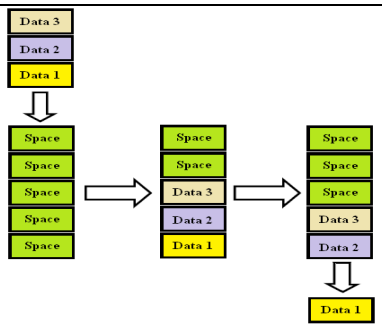

Fig.2 Operation of Synchronous FIFO

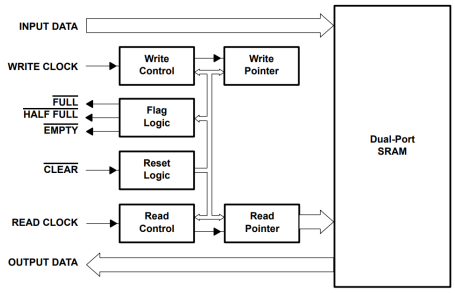

Fig.3 Block Diagram of FIFO with SRAM

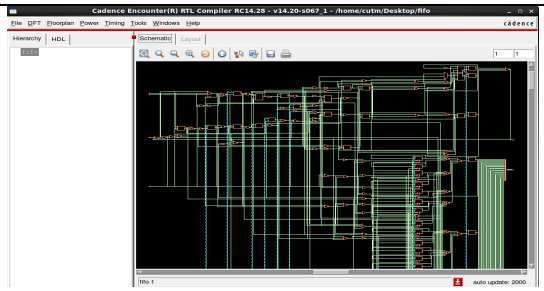

Fig. 4 RTL Diagram of FIFO Memory using RTL Compiler

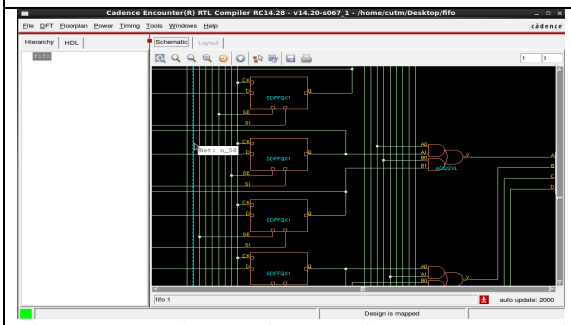

Fig. 5.a Internal RTL Diagram of FIFO Memory using RTL Compiler

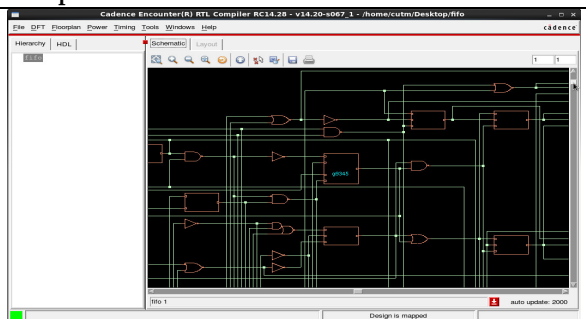

Fig. 5.b Internal RTL Diagram of FIFO Memory using RTL Compiler

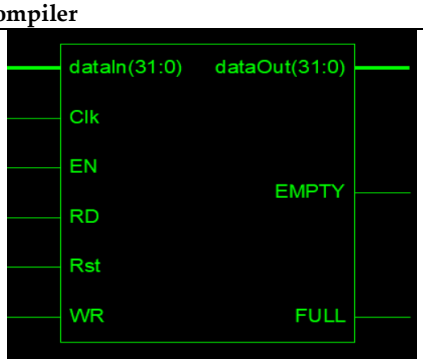

Fig.6 Top Module of 32-Bit FIFO Memory

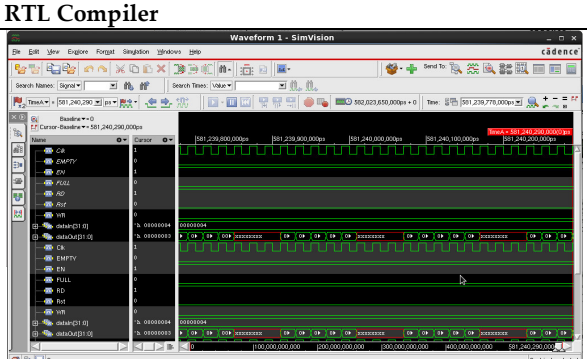

Fig. 6 Test Bench Simulation Waveform of FIFO Memory

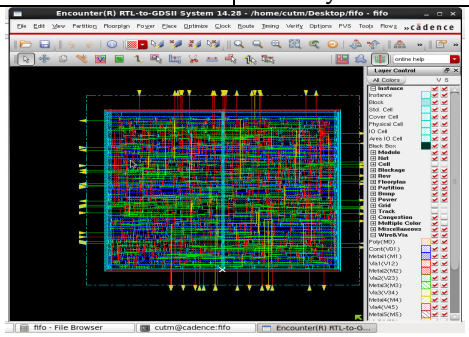

Fig. 7 Layout Design of FIFO Memory

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RESEARCH ARTICLE

ASIC Implementation of Halftone Image Converter

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ABSTRACT

A model of an algorithmic processor intended to perform the conversion of halftone pixel image utilizing Floyd Steinberg algorithm which enable to transform M-row N-column array of pixel array into a pixel of black &white having a resolution of N-bits. A technique called weighted average error is utilized to convert the given image having a resolution of N-bits to a halftone which is also called as 1-bit pixel. This is a substitute to image depiction, translation, storage, It provides an alternative for image depiction, rendering, storage and broadcast in place where unremitting tone of the image.

Keywords: Floorplanning, VLSI, Layout, Image processing, RTL

INTRODUCTION

In graphic and printing industrieshalf toning technique is widely used over a long period of time, traditional photograph method is replaced by digital techniques and it is well known that digital techniques scores over the traditional techniques. The attained halftone image can be portrayed easily in device ruled by binary gadgets. This makes the storage and processing of image easier. This technique lowers the image intensity for the best feasible reproduction and is widely used in printing factories. It is found that unremitting tone display causes discrepancy between representation and portraying ability as it encountered with constraints such as low cost, minimal system complexity and bit resolution is low [1-2]. It also lowers the depth of bit which makes it optimal for Error resilient transmission. Halftone image in mass printing media is produced the technique of screening. Prior to the era of digital images distinct photographic methods were used to perform the disruption of gray images into discrete points. [3]

The historic techniques basically use the screening in which before the exposing of screen camera, the screen of course-woven was suspended, breaking the light into dots pattern through diffraction effect and interruption together. By using the techniques of photo etching printing plates are being created.Resolution which is measured in lines per inch can be the amount of lines of dots in one inch, measured parallel with the screen's angle called the screen ruling. The resolution of a screen is written either with the suffix lpi or a hash mark; as an example, "150 lpi" or "150#".The higher the pixel resolution of a sourcefile, the greater the detail which will be reproduced. [4-5]

Floyd-Steinberg Algorithm

Floyd-Steinberg algorithm converts an image consisting of an N×M array of pixels, each having a resolution of pixel size, pixel_sizebit into an array having only black or white pixels, while incorporating a subjective measure of the quality of the image. The algorithm distributes to a selected subset of each pixel's neighbors the roundoff error induced by converting the pixel from a resolution of n bits to a resolution of 1 bit.The error distribution is calculated based on selected neighbors weighted average errors. The error distribution of neighbors received by a pixel which is used to calculate halftone pixel value (i,j) of the cell of N×M array with its origin value. The Data flow graph is obtained from the above relation that holds for each cell. Data flow graph nodes execute the conversion of pixels according to the following Pseudo code [6] The average error E_av can be expressed as

$$E\_av = (w_1 * e[i-1, j + w_2 * e[i-1, j-1] + w_3 * e[i, j-1] + w_4 * e[i+1, j-1]) / w_T \quad (1)$$

Where,

w_1, w_2, w_3, w_4 are the weights

$/w_T$= Total Weight=$w_1+w_2+w_3+w_4$

From the weighted average the corrected pixel value (CPV) is calculated as below

$$CPV = PV[i, j] + E\_av \quad (2)$$

According to the threshold value of CPV, CPV_threshold . Thus

CPV_round=0 if CPV<CPV_threshold

Else

CPV_round=CPV_max

For a 8 bit resolution image the CPV_max=255 and CPV_threshold=128

The halftone pixel value (HTPV) is formed and the error is saved as below

HTPV=0 if CPV_round=0

Else HTPV=1

Error [n, m] =CPV-HTPV

Sequentially the pixel array can be update by updating the row or column using nested loop program. The algorithm for sequential updating the pixels is executed using Verilog.

Implementation of Halftone Image Converter in Cadence

Verilog Code has been implemented to obtain all the top modules in cadence platform. It follows following tools to obtain both front end and backend result

- To Run Simulation: NCLAUNCH tool is used. Using this tool with implementing the test bench code the simulation result is obtained
- To Obtain RTL: RTL compiler tool is used for obtaining the RTL schematic of the design
- Synthesis Part : This section consists of converting RTL to GDSII , floor plan, power plan, placement, routing , pre and post timing analysis

RESULTS AND DISCUSSION

RTL Diagram: Using Encounter tool the RTL of the halftone image converter is obtained as shown in fig.1 and 2

Timing Analysis: For the proposed design the timing conditions is verified and it is found that it meets the timing requirements. The delay due to gates has been found as 25.734ns and the delay due to routing wires has been found as 24.82746ns. Thus the total time delay of converter has been found as 50.561ns

Cell Report: After compilation of RTL using RTL compiler the number of cells of each module and power is obtained. It has been found there are total 23,437 number of equivalent gates are available. When implemented with Xilinx ISE it has been found there are 2,129 number of 4 inputs LUT among which 2,004 number is used as logic, 436 number of bonded input-output blocks.

Backend Design: For backend design the RTL is converted to GDSII by using ENCOUTER tool. Here netlist is imported to obtain GDSII. In this part , floor plan, power plan, placement, routing , pre and post timing analysis is being done and the layout of halftone image converter is obtained and shown in the fig.4.a and 4.b

CONCLUSION

In this work an algorithmic processor intended to conversion of halftone pixel image utilizing Floyd Steinberg algorithm which enable to transform M-row N-column array of pixel array into a pixel of black &white having a resolution of N-bit. To begin with here an ASIC implementation of the converter is performed and the attained result is successfully verified at frontend as well as back end.It has been found there are total 23,437 number of equivalent gates are present.

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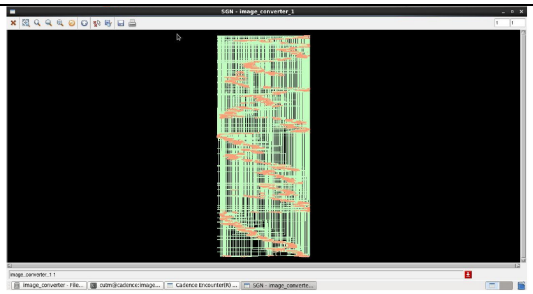

Fig.1 RTL Diagram of Halftone Image Converter

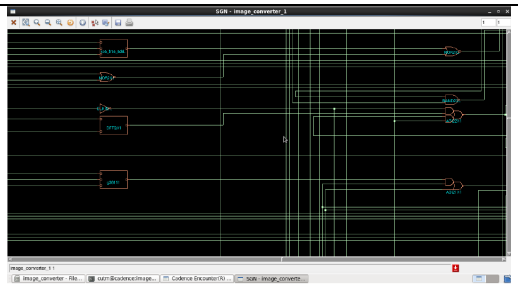

Fig.2 Internal RTL Diagram of Halftone Image Converter

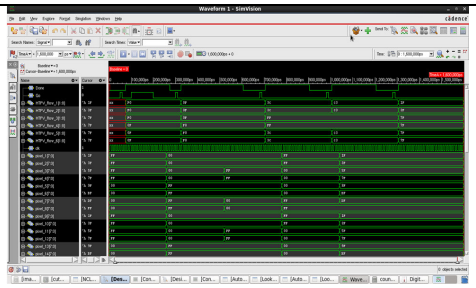

Fig. 3.a Testbench Simulation Waveform

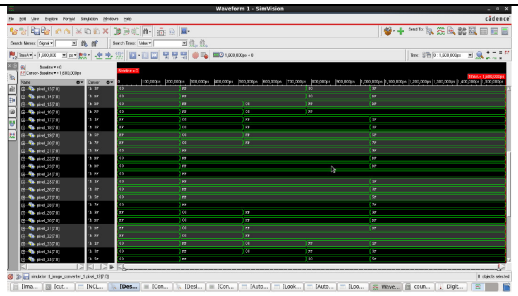

Fig. 3.b Testbench Simulation Waveform

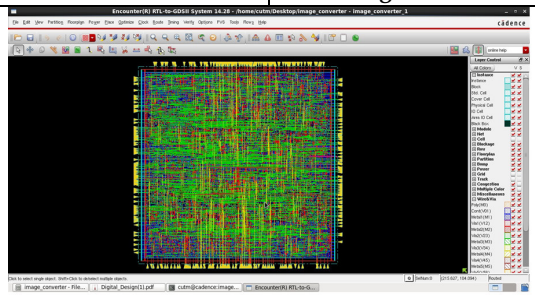

Fig. 4 Layout of Halftone Image Converter

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RESEARCH ARTICLE

Design and Implementation of Approximate Adder using Cadence

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ABSTRACT

Using the concept of Approximate computing the intricacy, delay and chip area can be reduced by permitting certain relaxation in output for inputs of few combinations. The minimization of circuit intricacy can be achieved by diminishing the population of components. In this work an approximate and exact Ripple carry Adder (8-bit) is designed using cadence. In order impinge approximate into the design a logic minimization technique is employed. Further, in order to validate the capability of the approximate adder two images are added with approximation and exact technique. Basically, a bitwise pixel addition of two images is performed using approximate and exact addition technique and it is observed that both the images are comparable.

Keywords: Ripple, performed, technique, area.

INTRODUCTION

Approximate computing is technique of computation which yields a conceivably non-exact result rather than a assured exact result and can be utilized for bids where approximate result is suffice to meet its purpose. This technique lowers the die area as well as delay and power consumption with a minimal negotiation with accuracy [1,2]. In literature techniques viz. cell minimization, truncation and logic minimization are widely utilized. In cell replacement method the module with more intricacy is substituted by its inferior circuit intricacy termed as approximate circuit, as result of which aberration in the anticipated output is observed and length of the critical paths is lowered. Another technique is truncation technique, where many versions of approximate adder circuit are designed by truncating the propagation of carry to higher blocks aimed at minimizing the delay; thereby achieving higher speed performance [3]. In segmentation method the modules with lower noteworthy blocks with approximate modules. Where as in order to lower the intricacy of the logic minimization method is used where bits of the

Karnaughmap are toggled thereby declining the complexity at the gate level. In this work a CMOS based approximate and exact adder is designed employing logic minimization method by using approximate SUM and CARRY expression, which lowered the number of gates [4].

METHODOLOGY

Verilog Code has been implemented in order to design the 8-bit Approximate and Exact adder.It follows following tools to obtain both front end and backend result:

- Approximate adder is proposed by incorporating intentional error in to the SUM and CARRY column of the truth table and the expression of SUM and CARRY is determined by minimizing the Karnaugh map.
- To Run Simulation: NCLAUNCH tool is used. Using this tool with implementing the test bench code the simulation result is obtained
- To Obtain RTL: RTL compiler tool is used for obtaining the RTL schematic of the design
- Synthesis Part: This section consists of converting RTL to GDSII, floor plan, power plan, placement, routing, pre and post timing analysis.
- Image processing studies is done using MATLAB simulation tool.
- Finally, approximate and exact addition of pixels is done using MATLAB.

APPROXIMATE ADDITION

The expression for the SUM and CARRY of the exact full adder is listed below in eq. 1 and eq.2

$$SUM = A \oplus B \oplus C \quad (1)$$

$$CARRY = AB + BC + CA \quad (2)$$

The minimized expression for the approximate adder is listed in eq.3 and eeq.4:

$$SUM = \sim AC \mid BC \quad (3)$$

$$CARRY = \sim AC \mid AB \quad (4)$$

The resultant sum and carry expression of Approximate and exact adder is achieved by deliberate incorporation of error in the sum and carry column of Approximate adder.

RESULTS AND DISCUSSION

RTL Diagram: The RTL of the Exact and Approximate 8-bit Ripple carry has been obtained using Encounter RTL compiler. It can be observed from the result that the RTL comprises of all the modules of the Ripple carry adder.

Simulation Waveform of the RTL: To validate the RTL obtained for the Approximate and Exact 8-bit Ripple carry adder has been simulated using RTL Compiler in cadence platform. The result validates the successful execution of exact and approximate adder.

Timing Analysis: For the proposed design the timing conditions is verified and it is observed to meet the requirements. The total time delay for the exact and approximate adder was found to be 304 pS and 171 pS.

Power analysis: The power consumption for the approximate and exact were found to be3441.650 nW and 4601.956 nW.

Cell Report: After compilation of RTL using RTL compiler the number of cells of each module and power is obtained. It has been found there are total 65.539 number of equivalent gates are available,

Backend Design: For backend design the RTL is converted to GDSII by using ENCOUTER tool. Here netlist is imported to obtain GDSII. In this part floor plan, power plan, placement, routing pre and post timing analysis is being done and the layout of approximate adder is depicted below.

Case Studies

In order to elucidate the capability of the designed Approximate ripple carry adder two images of identical size (m×n) is added which in turn produced a new image of the original size. 512 x 512 *cameraman image* is added with Rice image, it is found that the resultant image attained by approx. addition identical to the image obtained with exact addition. As it is shown in Fig.7

CONCLUSION

In this work we have successfully designed a8-bit Ripple carry adder (exact as well as approximate) using cadence virtuoso and investigated the power, delay and Area occupancy in the chip. In addition to that RTL synthesis and Layout of the chip is designed. It is found that our proposed design was area efficient as the number of components are reduced and it also resultingly reduced the power consumption and further due to the reduction of number components delay is also reduced.

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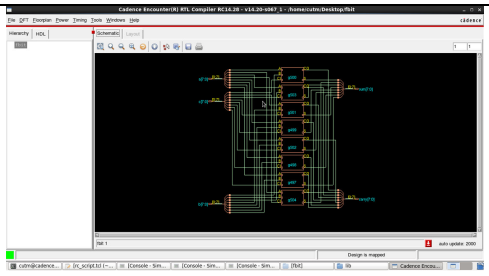

Fig.1 RTL Diagram of Approximate Adder

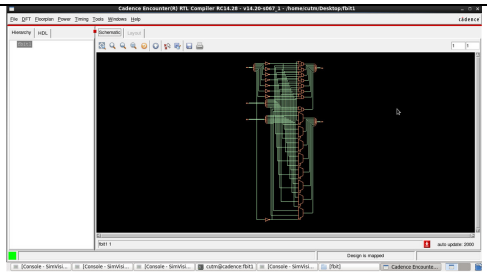

Fig.2 RTL Diagram of Exact Adder

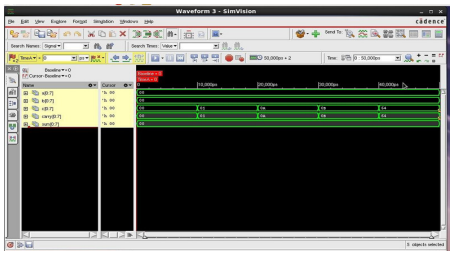

Fig. 3 Test Bench Simulation Waveform of Approximate Adder

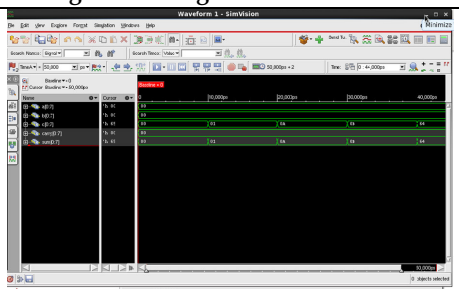

Fig. 4 Test Bench Simulation Waveform of Exact Adder

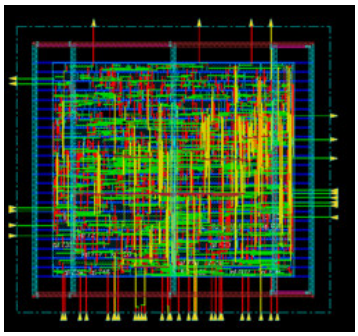

Fig.6 Layout Design of Approximate Adder

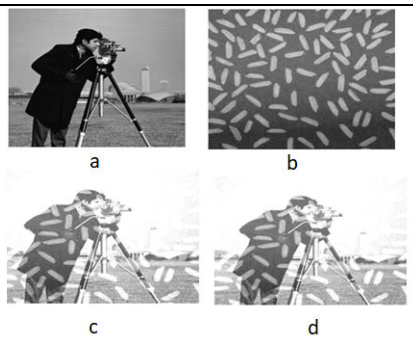

Fig.7 a. Camera Man Image b. Rice Image c. Exact Addition Image d. Approximate Addition Image

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RESEARCH ARTICLE

Design and Implementation of Wallace Tree Multiplier

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ABSTRACT

The foremost apprehension of VLSI engineers is power loss associated with the integrated circuits. It is basically an enhanced variety of multiplier which is found to be tree-based. The main feature of this multiplier is it uses the phenomenon of carry save addition which in turn lowers the latency. In this paper a 4-bit Wallace tree multiplier is designed using cadence EDA tool. The both front end and back end design of the Wallace tree multiplier is discussed in detail.

Keywords: engineers, phenomenon, multiplier, circuits

INTRODUCTION

One of the most important hardware blocks used in the high-performance digital systems are DSP, µprocessor and filters used for FIR applications. Many research groups have exasperated and attempted to build multipliers which exhibit attractive features such as expedite speedand minimalpower dissipation and dense implementations. Normally when we consider arithmetic circuits the key issue associated with them are area as well speed. Whenever it is attempted to enhance the speed there is always a increase in the die area. It is widely seen that the throughput necessity of the controls the structure of most efficient multiplier. In order to achieve an efficient multiplier structure primary objective is to decide the finest circuit structure configuration. The multiplication can be achieved by employing serial and parallel multipliers. [1-2]. The operation frequency of the DSP processor can be enhanced by increasing the speed of computation of the multiplier circuits. When the working of the Wallace tree multiplier is considered it performs the multiplication of a couple of unsigned integers. It basically comprises of an AND array for determining partial product. In order to add the partial productsa carry save adder is utilized and obtained product and the carry is allowed to proliferate adder in the ultimate phase of addition. [3-4]

DESCRIPTION OF WALLACE TREE MULTIPLIER

Process of Wallace tree multiplier goes through three basic stages such as partial product, partial product addition and final addition. In the partial product stage the long-hand multiplications are obtained using AND gates and all products are done simultaneously. Figure 1 shows an example of Wallace tree multiplier operation

DOT PRODUCTION OF WALLACE TREEMULTIPLIER

Fig.2 shows the dot production of Wallace tree multiplier. From the figure it can be seen that there are N number of multiplicand and multiplier bits are available. All the partial products are obtained in parallel and then by using suitable adders such as half adder and full adders the final addition is obtained. Fig.3 shows all stage operation in sequence [5].

DESIGN TECHNIQUES OF HIGH SPEED WALLACE TREE MULTIPLIER:

The numbers of addition operation required in conventional multipliers are high. Three partial product terms can be added at a time to form the carry and sum using the carry save adder. At the next level, the sum signal is used by the full adder. As the output carry of first full adder is passed to next full adder as a result the delay is coming to the design. For N number of rows the total delay is proportional to logarithmic value of 3n/2. The first and second stage of the multiplication is only depends on direct input using and array. However, the final value depends on the carry out value of previous stage for the intermediate higher stages.This operation is repeated sequentially for the consecutive stages. Finally, it can be seen that major cause of delay is propagation of the carry out from the previousstage to the next stage. In conventional Wallace Tree multiplier structure, the totalnumber of stages in the critical path sums up to 13. Each full adder used accounts for a latency of 2. Total latency of the whole structure gives a total of 26. The latency count gets increased by 1, when considered the and array, which results the total latency. The overall delay can be reduced using the technique shown in the Fig.4 and 5.

IMPLEMENTATION OF HIGH SPEED WALLACE TREE MULTIPLIER USING CADENCE

Verilog Code has been implemented to obtain all the top modules in cadence platform. It follows following tools to obtain both front end and backend result

- To Run Simulation: NCLAUNCH tool is used. Using this tool with implementing the test bench code the simulation result is obtained
- To Obtain RTL: RTL compiler tool is used for obtaining the RTL schematic of the design
- Synthesis Part : This section consists of converting RTL to GDSII , floor plan, power plan, placement, routing , pre and post timing analysis

RESULTS AND DISCUSSION

RTL Diagram: The RTL of the FIFO buffer has been obtained using Encounter RTL compiler. It can be observed from the result that the RTL contains all the modules of the designed high speed Multiplier. To validate the RTL design of Wallace tree multiplier the test bench code has been generated and compiled using RTL compiler and simulated wave form is obtained in SimVision as shown in the figure 7. The result shows the correctness of design of Wallace tree multiplier

Timing Analysis: For the proposed design the timing conditions is verified and it is observed to meet the requirements. The delay due to gates has been found as 8.812ns and the delay due to routing wires has been found as 7.116ns. Thus the total time delay of the designed multiplier has been found as 15.928ns which indicates the designed Wallace tree is faster in operation

Cell Report: After compilation of RTL using RTL compiler the number of cells of each module and power is obtained. It has been found there are total 4,728 number of equivalent gates are available. When implemented with Xilinx ISE it has been found there are 33 number of 4 inputs LUT among which 19 number is used as logic, 16 number of bonded input-output blocks.

Backend Design: For backend design the RTL is converted to GDSII by using ENCOUTER tool. Here netlist is imported to obtain GDSII. In this part, floor plan, power plan, placement, routing , pre and post timing analysis is being done and the layout of designed multiplier is obtained and shown in the figure8

CONCLUSION

A 4 bit Wallace tree multiplier with less computation time is designed. The multiplier design proposed here utilizes minimal count of full assisting in lowering the chip area. Here, 4-bit Wallace tree multiplier is designed using CMOS 180 nm process and using the cadence EDA tool. Beside front end and back end design is performed and successful working of the Wallace tree multiplier is verified.

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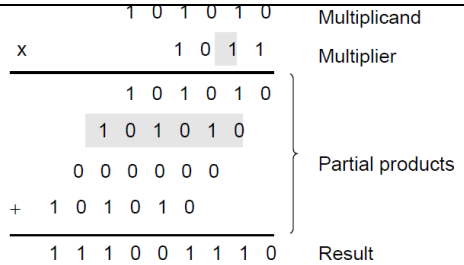

Fig.1 Example of Wallace Tree Multiplier

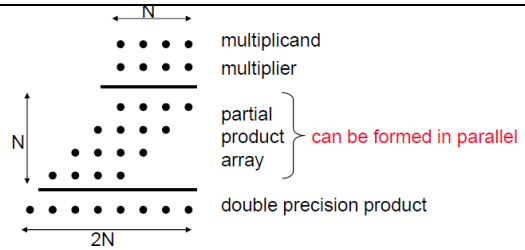

Fig.2 Dot Representation of Wallace Tree Multiplier Operation

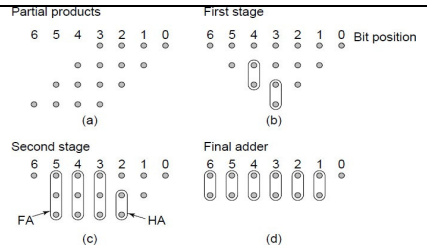

Fig.3 Stages of Wallace Tree Multiplier Operation

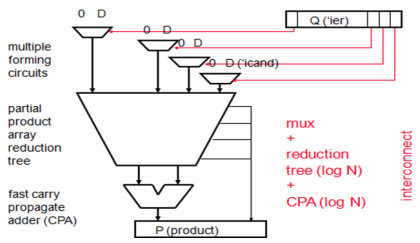

Fig. 4 Flow Diagram of High Speed Wallace Tree Multiplier

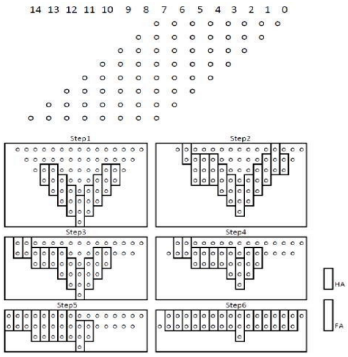

Fig.5 Steps Involved in Computation of Multiplication using High Speed Wallace Tree

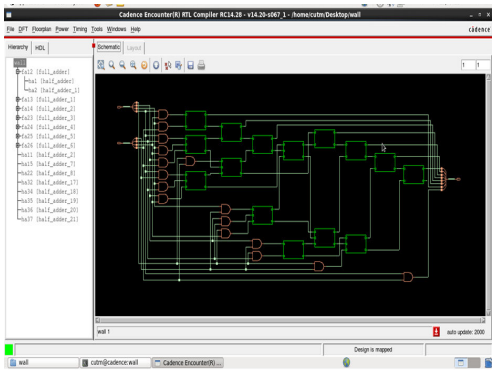

Fig.6 RTL Design of High Speed Wallace Tree Multiplier

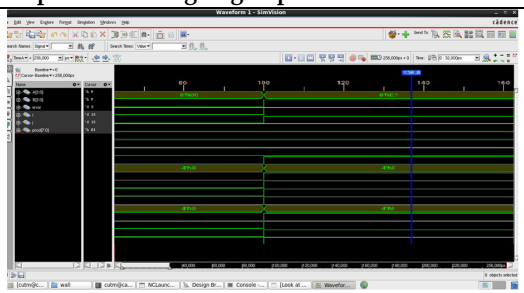

Fig.7 Testbench Waveform of High Speed Wallace Tree Multiplier

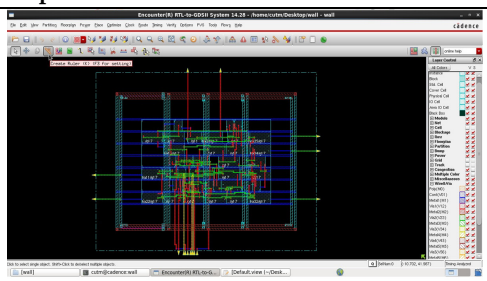

Fig.8 Layout Design of High Speed Wallace Tree Multiplier

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RESEARCH ARTICLE

Design and Implementation of UART Protocol

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ABSTRACT

In many applications is required to devices to communicate each other in order to share some useful data.Today there are many protocol are available each of them and their merit demerits and many application area.In between them one of the most powerful serial communications is UART(Universal Asynchronous Receiver Transmitter. In this paper UART protocol which is a serial protocol used for transmission of digital data is presented. It requires only two wire to communicate from source to destination.In UART protocol data format and transmission speed are configurable .Serial communication conveys a single bit at a time .Transmission of digital data can be achieved by sending all the data in a single wire so that over all communication cost and transmission speed is reduced to half as compared to parallel communication.In Asynchronous, communication no clock signal is required to transmitter to receive the data from source for synchronize the data but for synchronous communication clock signal is required for both transmitter and receiver for synchronize the data.In UART connection if two device are there i.e. device1 and device2, device1tx(transmitter)is directly connected to device2 (receiver) and then vice versa. Both ground should be connected directly device1 to device2. Due to no clock signal in asynchronous the all the communication is based upon UART baud rate of 9600bps .And one start bit and stop bit in each data bit here parity bit(optional bit) is used by transmitter for error detection. The work is implementedin HDL Verilog and verify by UVM using Xilinx ISE 14.0 and Questasim2.0.

Keyword: VLSI, Transmitter, Receiver, Data Transfer

INTRODUCTION

In order to receive and send data in serial mode a device called UART is used. It exchanges data in ASCIIformat where every alphabetical character is encoded into seven bits and sends as 8 bit data. While during the process of

transmission it squash 8 bit sub-word where the first bit is LSB where as stop bit is considered as MSB consequently building it to a format of 10 bit word.

Start	Data 0	Data 1	Data 2	Data 3	Data 4	Data 5	Data 6	Data 7	Stop

Transmitter of UART basically fetches the data in parallel format and instructs the UART to send in the format of data in serial. Similarly, receiver must perceive the data in serial style, strip of the start and stop bits, and store the data word in a parallel format. As it is well known that the working of the UART is asynchronous in nature receiver is not aware of what data it will receive a local clock is generated tosynchronize the transmitter as and when acceptance of start bit. When the process of transmission is asynchronous, the data can be sent without the reception of clock signal from the receiver. The transmitter and receiver agree on timing parameters in advance and special bits are added to each word which is used to synchronize the sending and receiving units. When a word is given to the UART for Asynchronous transmission, a bit called the "Start Bit" is added to the beginning of each word that is to be transmitted [1-3]. The job of start bit is to aware the receiver of the of what data word it is supposed to be sent and forcefully synchronized the clock of transmitter as well as receiver. Upon the sending of Start Bit, individual data bits of the words of the data are transmitted where first bit is the LSB. During transmission, the time of transmission of all the bits is exact and receiver "looks" at the wire at approximately halfway through the period assigned to each bit to determine if the bit is a 1 or a 0

UART CONNECTION DIAGRAM

The serial port of UART IS basically a 9 pin architecture, which provides asynchronous communication widely, called as RS-232. The UART component can be configured for Full Duplex, Half Duplex, Rx only or Tx only versions. Configurable buffers are provided in order to process receive and transmit data with the help of UART. In order to configure the UART by choosing proper BAUD rate, parity and number of start bits [4,5].
It indicates the Baud rate must be fixed. To support the UART variations commonly used, the component provides configuration support for the number of data bits, stop bits, parity, hardware flow control and parity generation and detection.

METHODOLOGY

The UART protocol has been implemented in Xilinx ISE 14.0 using Verilog HDL code. The Top module and RTL of both transmitter and receiver obtained after the synthesis. The UART protocol has been verified by using number of test cases in Questasim2.0 to validate the correctness of implemetnatio of UART protocol.

RESULTS AND DISCUSSION

RTL Diagram

The RTL of the transmitter and receiver has been obtained using Xilinx ISE. The Top module of both transmitter and receiver is sown in Fig.2 and 3.The top module and RTL of transmitter is shown in the Fig.2.aabd 2.b respectively. From the top module of transmitter it can be observed that the inputs to the modules are clock, load, reset, shift and select. The select input basically control the whether the operation is load or shift and the outputs of the transmitter module are CS, Txd and ready. The RTL of the receiver has been obtained using Xilinx ISE. The Top module and RTL of receiver is shown in Fig.3.a and 3.b

Simulation Waveform

To validate the RTL of both transmitter and receiverdifferent test cases are taken to verify the working conditions,

Test Case 1:D_{in} and parity_e_o randomized with constraints reset==1'b1;tx_enable==1'b1, here reset=1 that means signals are in ideal conditions, this test case verifies the reset signal

Test Case 2: D_{in} and parity_e_o randomized with constraints reset==1'b0;tx_enable==1'b0, this test case shows, here tx_enable==0, means no transmission operation occurs. This test case verify the tx signal.

Test Case 3: D_{in} and parity_e_o randomized with constraints reset==1'b0;tx_enable==1'b1, this test case shows, here we are sending one data frame and all signals are transmitting as well as indicates the transmission operation of UART.

Test Case 4:D_{in} and parity_e_o randomized with constraints reset==1'b0;tx_enable==1'b0 here we are repeated this process five times successfully.

Test Case 5:D_{in} and parity_e_o randomized with constraints reset==1'b1;rx_enable==1'b1, this test case shows, here reset=1 that means signals are in ideal conditions, this test case verify the reset signal

Test Case 6:D_{in} and parity_e_o randomized with constraints reset==1'b0;rx_enable==1'b0, this test case shows, here rx_enable is low, means no data will be recieved. This test case verify the rx signal.

Test Case 7:D_{in} and parity_e_o randomized with constraints reset==1'b0;rx_enable==1'b1, this test case shows, here we are receiving one data frame as well as indicates the receiver operation of UART

Test Case 8:D_{in} and parity_e_o randomized with constraints reset==1'b0;rx_enable==1'b0 here we are repeated this process five times successfully.

CONCLUSION

In this paper the UVM frame was presented. The "Top". Inside the "Top" was created along with "Environment", "Read Agent", "Write Agent" and "Test". After successfully creating the UVM frame the logic was developed according to the assigned UART protocol. The logic for driving the signal to interface and for extracting the signal from interface and sending it to scoreboard while monitoring it was also developed. The results obtained validate the successful implementation of UART protocol.

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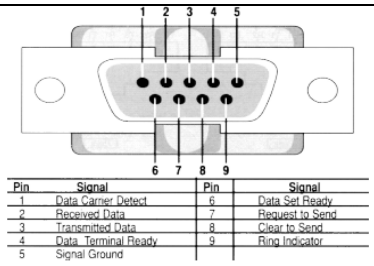

Fig.1 UART Connection Diagram

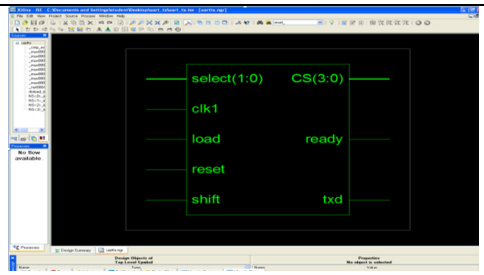

Fig.2.a Top Module of Transmitter

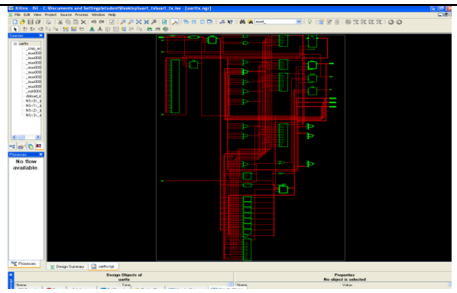

Fig.2.b RTL Diagram of Transmitter

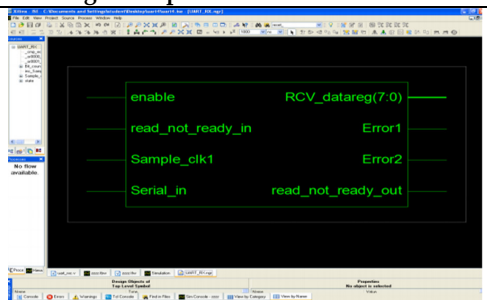

Fig.3.a Top Module of the Receiver

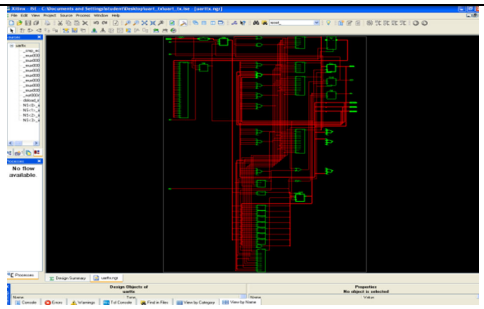

Fig.3.b RTL Diagram of Receiver

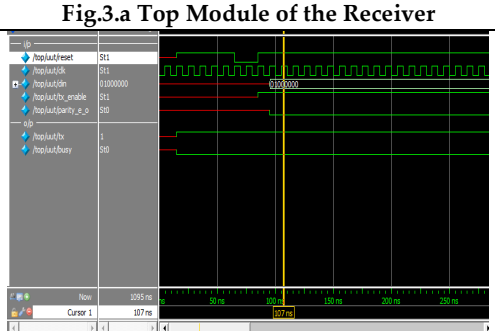

Fig.4 Simulation Waveform of Test Case: 1

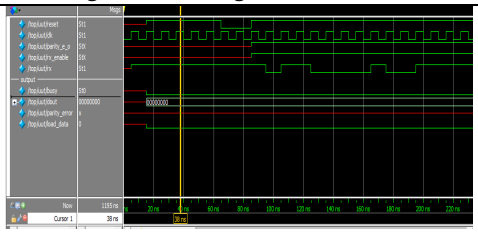

Fig.5 Simulation Waveform of Test Case: 2

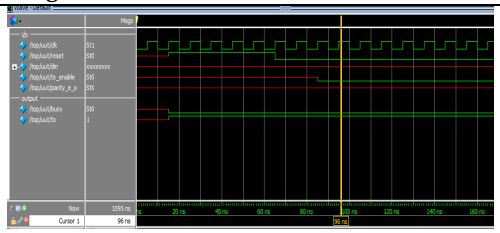

Fig.6 Simulation Waveform of Test Case: 3

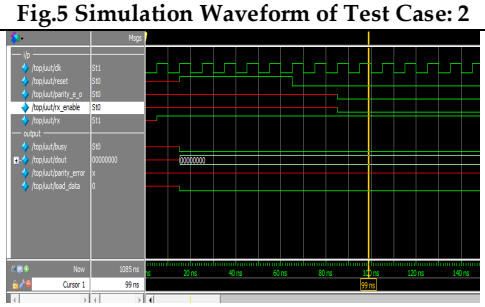

Fig.7 Simulation Waveform of Test Case: 4

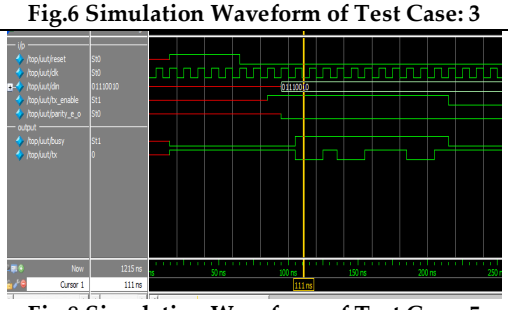

Fig.8 Simulation Waveform of Test Case: 5

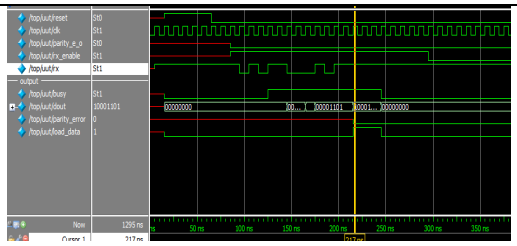

Fig.9 Simulation Waveform of Test Case: 6

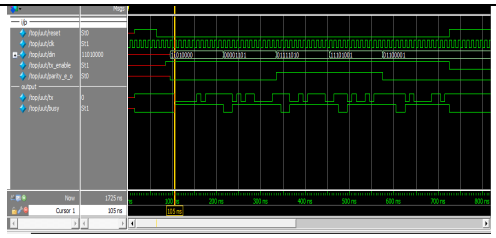

Fig.10 Simulation Waveform of Test Case: 7

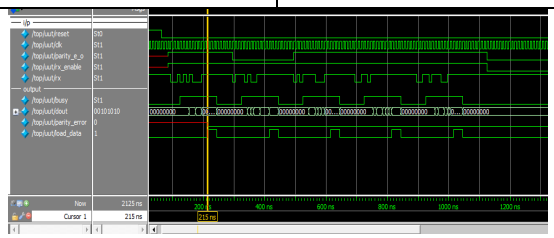

Fig.11 Simulation Waveform of Test Case: 8

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RESEARCH ARTICLE

Design and Implementation of Memristor based Sequential Circuits

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ABSTRACT

Memristor (Memory-Resistor) are two terminal device of nanometer size, they lie in between nanodevices and electronics therefore it is a type of nano electronic device. In this work Verilog A model of memristor is used to design sequential circuits using hybrid memristor and CMOS transistor. The designed digital logic circuits were found to work with proper functionality. As the size of the device lies in nanoregime and as it can employed as memory as well as logic element, hence it would provide the privilege of thinking beyond Von-Neumann Architecture.

Keywords: Memristor, MRL, Non-volatile Memories, RRAM

INTRODUCTION

Memristor (Memory-Resistor) are two terminal device of nanometer size, they lie in between nanodevices and electronics therefore it is a type of nanoelectronic device. The common analogy for the esistor is a water pipe, where the flow of water is similar to the flow of charge (electric current) and pressure applied at the input of the pipe is analogous to the voltage applied. Memristor is a pipe where the diameter of the pipe dilates when water flows in one direction and shrinks when the water flows in the opposite direction.As the name "memory resistor" implies it is a non-volatile random access memory (NVRAM) [1-3]. This class of devices on switch off, the data is not lost. It is widely used in the application of Artificial Intelligence, which can be used to artificial brain mimicking the functionality of the animal's brain in a system-on-chip. This behaves like an artificial synapse and neuron can be built with aid of it [4,5].

METHODOLOGY

In this work a Verilog A model of memristor is used to create a symbol of the memristor in the cadence virtuoso tool. Once the symbol is created it is instantiated into the virtuoso window and it is utilized to design Memristor sequential circuits.

RESULTS AND DISCUSSION

Previously few works has been reported on the application of Memristor in combinational circuits. Here a case study is performed in order to test the application of Memristor in sequential circuits. The working of SR and D Flip-flop is verified by utilizing the Memristor based NAND gates are presented in this section.

Memristor Based SR Flip-Flop

This is otherwise termed as SET-RESET Flip-flop. Initially assume that q=0, qbar=1 and clock (clk) =1. When both the inputs S and R are "0", it is observed that there is no change in the value of q and qbar. The Fig. 2 depicts the above case. It is called as SET-RESET Flip-flop because the value of q depends on the input S and R.If the input S is high then q=1, which implies that the Flip-flop is in SET condition. The Fig.3 depicts the above case. If the input R is high and S is low then q=0, which implies that the Flip-flop is in RESET condition. The Fig.4 depicts the above case.When both S=R=1 it is an invalid condition as both the values of q and q' turns high which is practically impossible. The Table-I shows the truth table of SR Flip-flop.

Memristor Based D Flip-Flop

The D Flip-Flop is designed from the SR Flip-Flop by connecting both ends to the two ends of an inverter. It stores the data present in the D input at every positive edge of clock. It is otherwise called transparent latch as both the input and output are same. The Fig.5 represents schematic and Table-II represents the truth table of the Memristor based D Flip-Flip. For the device to operate properly D input must be stable for some time before the positive edge of the clock. This time period is defined as setup time. Even after the positive edge of the clock for a small period of time the latch holds the input, so that the input signal can be sampled properly. The above truth table is verified in Fig.6 and Fig.7 for the input of "0" and "1" respectively.

CONCLUSION

In this work a Verilog A model of Memristor prepared by incorporating the Verilog A code into the Cadence Virtuoso. The design was found to be power and energy efficient as it is designed using area and power efficient nanoscale memristor. This work paves the way for future implementation of memristor in logic design applications.

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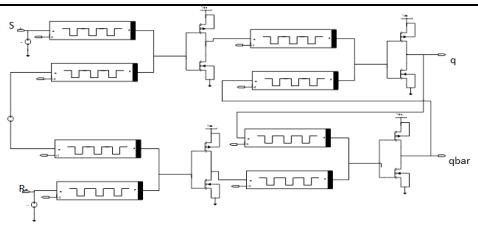

Fig.1 Schematic of Memristor based SR Flip-flop

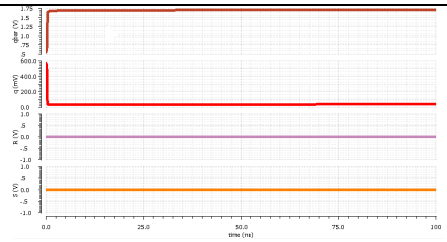

Fig.2 S=0 and R=0 case for SR Flip-flop

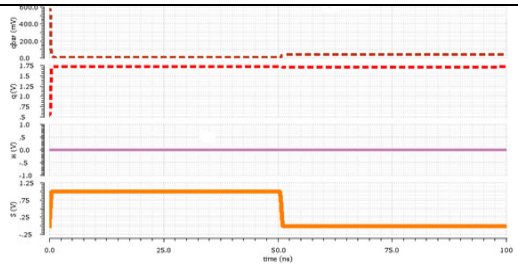

Fig.3 S=1 and R=0 case for SR Flip-flop

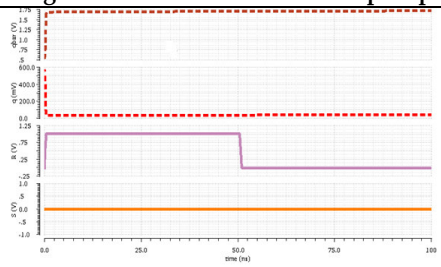

Fig.4 S=0 and R=1 case for SR Flip-flop

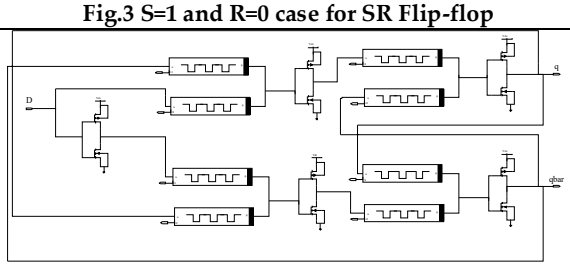

Fig.5 Schematic of Memristor based D Flip-Flop

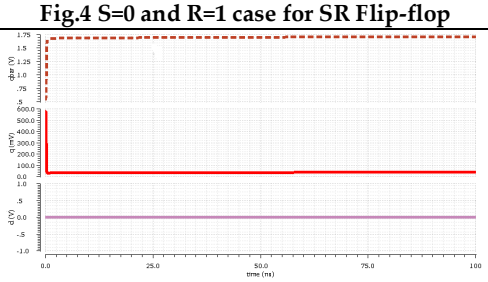

Fig.6 D = 0 case for D Flip-Flop

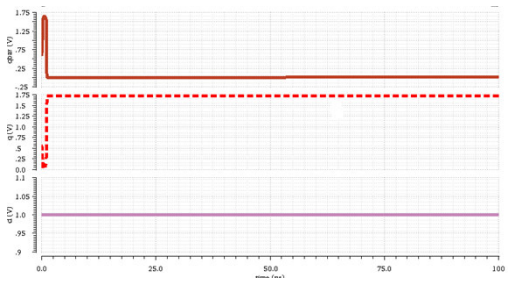

Fig.7 D = 1 Case for D Flip-Flop

TABLE-I: Truth Table for SR Flip-Flop

Clk	S	R	Q_{n+1}	Q'_{n+1}	State
1	0	0	Q_n	Q'_n	Hold
1	0	1	0	1	Reset
1	1	0	1	0	Set
1	1	1	1	1	Invalid

TABLE II: Truth table of D-type Flip-Flop

Clk	D	Q_{n+1}	Q'_{n+1}
1	0	0	1
1	1	1	0

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RESEARCH ARTICLE

Barcode Detection using Computer Vision

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ABSTRACT

Worldwide everything becomes digitize with the evolution of digital technology. The digitization help to reduce complexity of access anything or anybody, even due to digitization everything can be digitally store. Barcode system is one of the kinds which assigned to each category of product to make easy to maintain database of product as well as access all the information about the product. In this paper a method has been proposed to detect bar code on a product. This process is very necessary before recognizing the bar code. The processes of detection involve segmentation and morphological operation to detect the line pattern on an scene image. The method has been tested in different category of barcode and giving around 95 % result.

Keywords: barcode, computer vision, segmentation, morphology

INTRODUCTION

In the recent era, everything becomes digitized, with the help of evolution in digital world every where the system becomes digitized starting from online purchasing of goods to offline purchase of good. Even the house hold grocery items have some digital information in the seller digital computer. Due to this digitization the consumption of time for completion of a process get reduced, even the human effort also getting reduced. In place of human being the computer system are getting replaced. Even human brain can perform any mistake, but the trained system work accurate as well as faster. Any products which are digitally available to the consumer should have digital information available in terms of barcode. When products are available in a store the store owner should keep a rack of the product. The product data base is maintained to maintain the database and delivery of the product with faster billing to costumers. The store manager coded each product with a bar code in which the details about the product embedded into it. Even in the industry where the product manufactured also made such barcode to each product during manufacturing process. The barcode contain all information related to the product [1]. By this process each product can be differentiated form each other even if similar products can be categorized to separate group. The

main part of the system is the delivery to customer, during the process the each product need to billed using a bar code scanner [2, 3]. The barcode scanner work is to detect barcode and scan it and extract the information embedded with it which called as barcode recognition. But before recognition, the most important part is to detect the location of barcode for the system. This paper focuses on a simple approach to detect the barcode using computer vision and image proessing technique.

Computer Vision and Image Processing

Computer vision is a field of science and technology which train the machine to visualize the real world like human eye and took decision [4]. It performs the task with the help of devices like digital camera and some image processing technique. The image processing is the technique to extract information from the capture through some processing algorithm. The image processing technique involves different methods like image acquisition, enhancement, segmentation etc.

Barcode

A barcode is generally a visual of black and white pattern. This is a kind of method to represent information in visual graphics form which can be understood by machine. The barcode patterns are black and white pattern of parallel line or random pattern. The barcode first invented by NJ Woodland and B Silver and patented in US. And it took years to make the bar code commercialized. The barcode are broadly classified into 1D (one dimensional) or 2D (two dimensional barcode.). Universal Product Code (UPC) code, EAN Code, Code39, code 128, Code39 are some types of 1D type bar code where as QR Code, data matrix code, Aztec Code are some types of 2D type barcode[5]. The UPC code was first developed to code the products, but now days it has been spread to almost every filed even in the identification card also include QR code.

Bar Code Detection Methodology

Before extraction of the information from the bar code, the system has to detect the barcode after taking a picture through the digital camera. The detection of bar code methodology has been given as a flow diagram in figure 1.
The implemented method involves the following computer vision operation:

- Color conversion
- Image Segmentation (Gradient)
- Image Thresholding
- Image Morphology
- Contour Detection

As the capturing device follow the RGB color model, so the capture image through device like camera rae of RGB image. First the color image has been converted to gray scale image and the captured image become a mono chrome image..Segmentation is the process of subdividing the image into sub region, but line and edges detection are part of segmentation [6, 7]. The edge detection can be performed vertically as well as horizontally which detect both horizontal and vertical edges of the gray scale image. A barcode always has a very high horizontal gradient and a very low vertical gradient. So for bar code detection the vertical gradient is getting subtracted from horizontal gradient.

After the both the gradient detection, both the result get subtracted which form a gradient image. The resulted image has gone through an averaging operation to make the resulted image smooth via blurring operation. The smooth image has been thresholded using binary thresholding method, so that the resulted image becomes a black and white one. The thresholding operation will separate the image in to two segment based on the histogram. Image morphology is that operation which helps to extract structure of image for representation and description. Dilation and erosion are the two very basic operations under morphological operation. Dilation generally thicken the boundary where as erosion reduce the boundary width [6, 8]. But here both the operation used using a specific type of structuring element which fill the gap between bars and also remove the unwanted region and leaving behind the

significant region as contours.. Finally all the contours of the morphological image have been determined and the larger counter will be detected and kept within a rectangular bounding box [9]. The larger contour represents the barcode region. The result after each step is shown in figure 1-9 The method of barcode detection has been implemented on varieties of barcode images printed on items like books, cosmetics, food products etc. The resulted bar code detected images have been shown in figure 11. The method is very simple and it working fine with most of the image , but some time it give false output which are due to effect of improper illumination.

CONCLUSION

In the digital era every product can be digitally accessible by coding with an barcode. The information about the product can be easily access by a barcode scanner. The vital task of a barcode scanner is to detect the barcode. This paper implement a image processing approach based on segmentation and image morphology to detect the bar code region. The method has been tested among different varieties of producyt image and giving aroung 95% of accurate result but in some cased due to poor illumination the detect giving false result. This method is only applicable for two dimensional barcode. In future the complete barcode detection as well as recognition can be implemented using the computer vision.

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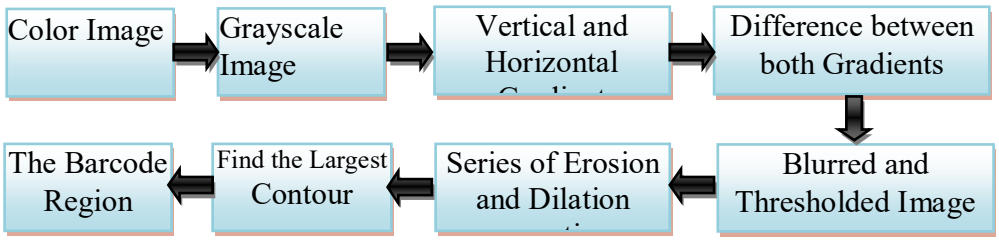

Figure 1:. Flow diagram for barcode detection

Figure 2: Captured RGB Image

Figure 3: The Gray scale image

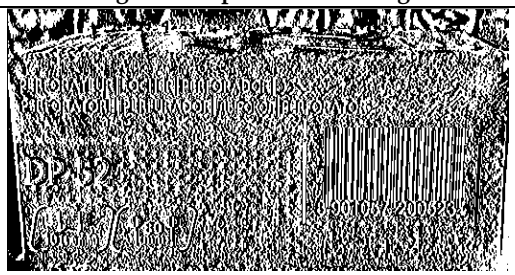

Figure 4: The vertical edge detected output

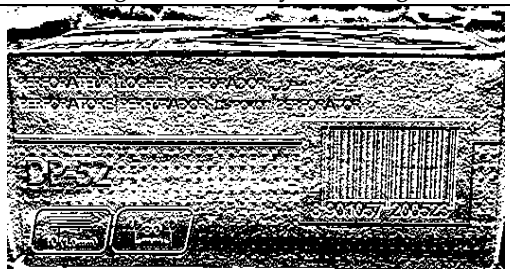

Figure 5: The horizontal edge detected output

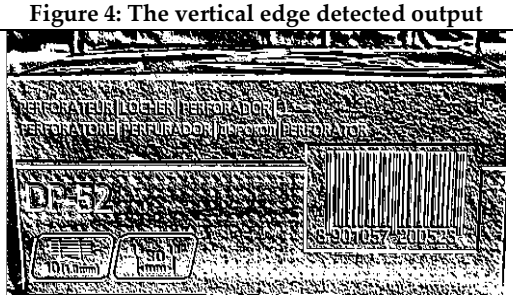

Figure 6: The resultant gradient image after subtraction

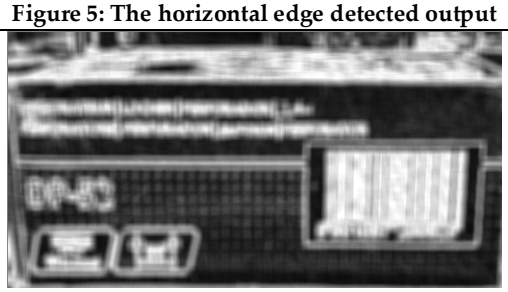

Figure 7: The blurred image

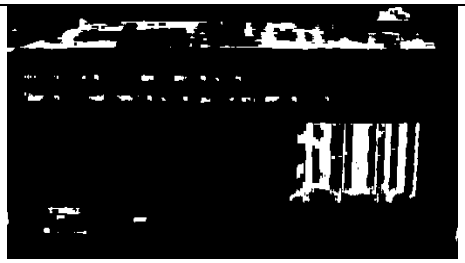

Figure 8: The thresholded Image

Figure 9: The dilation followed by erosion

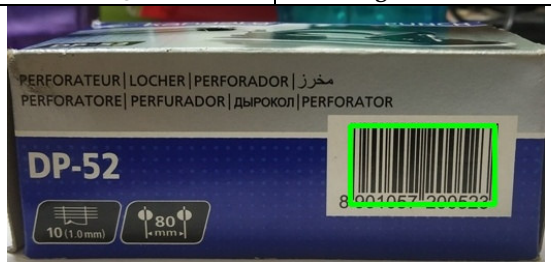

Figure 10: The barcode region enclosed by bounding box

Figure 11: Result for barcode detection for various product images

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RESEARCH ARTICLE

Physical Modeling of Electronics Circuit using Simulink for Online Class

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ABSTRACT

In present scenario, the physical classes is quiet not possible, so every where online classes are preferable by the institutions. Most of the electronics designs are used using the physical components and the virtual simulation of such electronics design is necessary for online classes. For the simulation of such design MATLAB and Simulink tool is a well structure and organized available tool. The MATLAB deals with high level complex computation where as simulink deals with graphical programming for modeling of system. This paper presentenced a virtual simulation of electronics circuit (full wave bridge rectifier) for online tutorials though physical design using simulink tool. The simulation result has been compared with the theoretical concept to verify the correctness of the model design in simulink. This type of digital simulation of physical system will be beneficial for online classes. A library called Simscape has been used for physical modeling of the electronics system.

Keywords: physical design, simulink, Simscape, virtual simulation

INTRODUCTION

The electronics circuits can be developed physically using the physical components designed on a breadboard and can be tested with real time with application of voltage. But in the current situation of world with effect of COVID 19, most of the institutes are focusing on online classes [1, 2]. The online classes can be more effective when the physical design can be performed with digitally through online. So the virtual simulation of the physical electronics circuit design is very much necessary. Even in the other way virtual simulation with provide ease of analyze the output for different set of parameter. So it is better to design any circuit virtually and simulate it prior to real world physical design. Even if the physical components not available then also different online virtual lab different electronics circuits can be developed.

In this paper simulink has been used for the digital simulation. Simulink is a tool combined with MATLAB and both the tool which are preferable for engineering simulation as well as physical design of dynamic system. It is vastly used tool worldwide across all discipline [3]. In this paper a bridge rectifier has been chosen as a basic electronics for virtual simulation. Simulink is a model based simulation tool based design environment. Basically it comes integrated with MATLAB developed by the company MathWorks. MATLAB has been developed for the high level computation where the simulink has been developed by physical modeling. Simulink is a kind of graphical pick and place based programming language for system modeling. Most advantage of the simulink is that it is used for analyzing the dynamic system in an organized way. The simulink has different library of blocks sets like control system toolbox, communication system tool box, simscape, state flow etc. It also include basic block set library like continuous, discontinuous, sink, sources, Math operators etc. Simscape block set library used to create models of physical systems within the Simulink. Physical model can be implemented with physical inter connection which directly block diagram and other resources. More complex analysis can be possible with the Simscape library [4, 5].

Full Wave Bridge Rectifier

A rectifier is an electronics device which convert unidirectional to bidirectional signal or in simple word alternating current to direct current. This is again dived into two types: Half wave rectifier which can able to convert only positive or negative half cycle, where the second category is full wave rectifier which can able to convert both the half cycle into direct current. Actually the rectifier alone can't able to convert as pure dc rather it can be possible with the help of capacitor, inductor or combination of both filter. The full wave bridge rectifier is a combination of four semiconductor PN side arrange in a bridge connection [6, 7]. Te arrangement is such a way that it can able to convert both the half cycle in to a positive wave form. The circuit diagram with all the connected components with the output waveform shown in figure 1-2.

Experimental Implementation with Simulink

The Simscape library contain some foundation library as well as Electronics, Hydraulics, Mechanics and power system related physical block set with some utility block set. The semiconductors components require to design the full wave bridge rectifier are available in Electronics section called as *SimElectronics*. The following block sets required to designed the circuit are shown below with their location where available

- Semiconductor diode: Simscape/SimElectronics/Semiconductor Devices/Diode
- AC Voltage Source: Simscape/SimElectronics/Sources/Voltage Source
- Electrical Elements:
  Simscape/Foundation Library/Electrical/Electrical Element/Capacitor
  Simscape/Foundation Library/Electrical/Electrical Element/Resistor
  Simscape/Foundation Library/Electrical/Electrical Element/Ideal Transformer
  Simscape/Foundation Library/Electrical/Electrical Element/Electrical Reference
- Utility block-Simscape/Utilities/PS-Simulink Converter
- Simscape/Utilities/Simulink-PS Converter
- Simscape/Utilities/Solver Configuration

The following steps can be followed to designed the physical modeling as a simulink model using Simscape
Steps:

1. Create a new model on simulink
2. Select the required block from the respective section of the package.
3. Add them to the model
4. Place the component at appropriate place with proper orientation
5. Connect the block as per the circuit diagram to get the bridge rectifier circuit model

For the complete functionality of the circuit design, it needs to connect some more blocks. The voltage sensor will be connected at output load will receive the physical output values which can't be shown there directly. It has to be connected to a scope through a PS-Simulink converter, which convert the physical output to a simulink output. Now through a scope it can be visualized. Each physical model designed in Simscape block diagram requires solver settings information for simulation. The Solver Configuration block specifies the solver parameters that your model needs before you can begin simulation.

Then after set the model configuration parameter, the model has been executed, the execution will be performed for a specific time mentioned during the configuration parameter. The output graph can be shown through the scope. The designed model first simulated without using the capacitive filter and the resulted graph able to convert both the cycle into positive wave form, but the output is not the proper dc. It is a kind og pulsating dc due to presence of some ripple. In the second phase the model has been simulated with a connected capacitive filter at the output. The result achieved was a perfect dc. This is due to the fact that the capacitors bypass the ac component to ground and all dc components will be passed to the load as the capacitor connector parallel to the load. The designed circuit and the simulation result have been shown in figure 3-6.

CONCLUSION

The paper presented the implementation of electronic circuit using the Simscape physical modeling library of simulink. This library greatly helps in multi domain physical system. For modeling and simulating electronics circuit a full wave bridge rectifier has been chosen. The model simulated in two cases one with the use of capacitive filter and another without using the filter. The output signal than compared with the theoretical concepts of the full wave bridge rectifier, it performing 100% same result as pet the theoretical concept. The digital implementation of the circuit design and simulation has a great impact on the online classes, now it can be proved that even online classes has the experimental simulation of hardware circuit through the digital representation. In future it can be extended to design OPAMP based circuit such as differentiator, integrator and oscillator.

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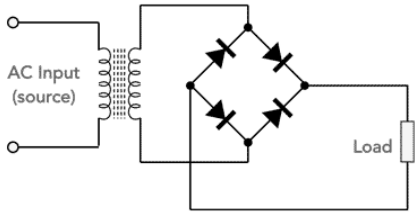

Figure 1: The connected circuit diagram of Full wave bridge rectifier

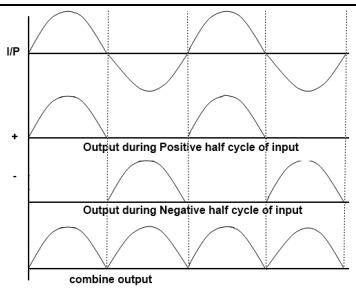

Figure 2: Output wave form of Full wave rectifier

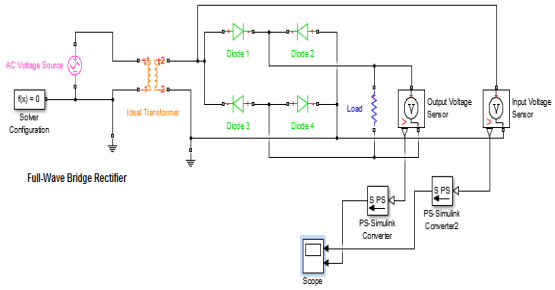

Figure 3: Simulink model of full wave bridge rectifier (without capacitive filter)

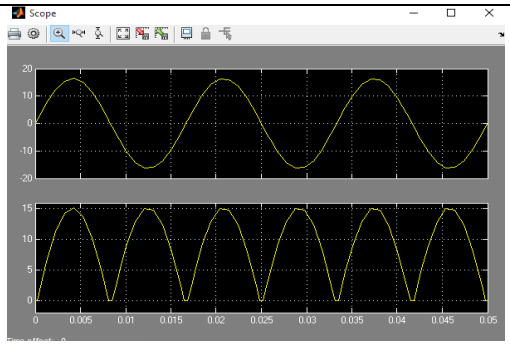

Figure 4: Output wave form of full wave bridge rectifier (without capacitive filter)

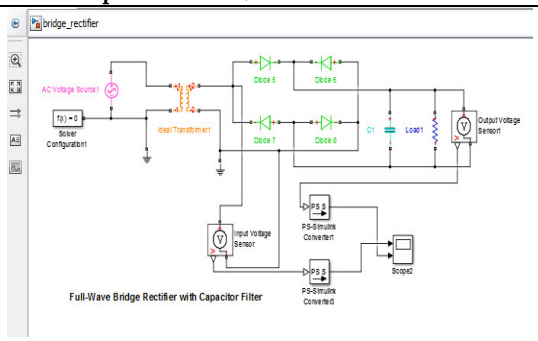

Figure 5: Simulink model of full wave bridge rectifier (with capacitive filter)

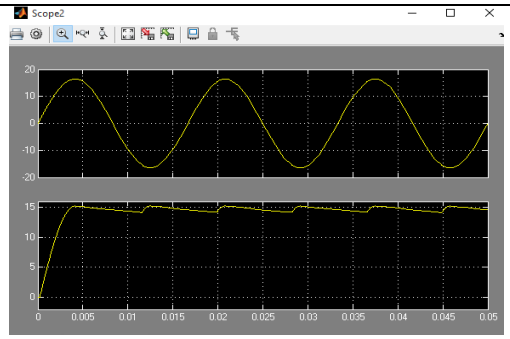

Figure 6: Output wave form of full wave bridge rectifier (with capacitive filter)

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RESEARCH ARTICLE

A Comparative Design and Analysis of Broadband Rectenna application to wireless Energy Generation

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ABSTRACT

A broadband rectenna is designed and simulated which is applied to wireless energy Generation. The Rectenna is designed using two software tools named as HFSS and ADS. After the design, they are mapped into same platform to compare their result. In this paper, the ractifying antenna designed is operated at 2.4GHz which consist of spilled four element array structure, series fed of dual element array and antenna parts Specially for the near field study this array structure is adopted to adopt different power density. To minimize the substrate loss, squeezed small-shape air supported microstrip antenna is designed. In this paper, the capacitance is substituted by microstrip line in the form of dc pass filter and the diode in the rectifying circuit is connected in sequence. The energy conversion efficiency from RF energy to DC electrical energy reached 80.25% by maintaining 20.85 dBm and 3501 ohm resistive load through repetitive experiment respectively. So maximum 18.55 volt of DC output voltage is observed and noted during simulation. The entire circuit is designed and can be expandable to huge scale to produce mass electrical energy for any type of wireless power transmission.

Keywords- Rectenna; parameter; time domain; bandwidth; Design; application

INTRODUCTION

In recent years, Wireless technology and device is more and more demanding due to its more compatibility and portable in nature. The great revolution occurs just starting of 21st century when global system for mobile communication starts its peak. Many types of antennas are optimised in miniaturization and shape compactable to cell phone and telecom network fro range of 890 – 960 MHz From that year cell phone dimension becomes smaller and smaller .Till now also researchers are waiting for smallest size of mobile in this world. The other bandwidth are

digital communication system from 1710MHz to 1880 MHz , the personal communication system from 1850MHz to 1990 MHz) and the universal mobile telecommunication system from 1920MHz to 2170 MHz which becomes essential day by day. Planar antennas are also very eye-catching in telecommunication instruments for wireless local area network systems at resonant frequency of 2.4 GHz which have ranges of 2400MHz – 2484 MHz and resonant frequency of 5.2 GHz which have ranges of 5150MHz– 5350 MHz bands respectively.

Design and analysis

Rectenna antenna model design and analysis

Here, A Rectenna is designed using HFSS and simulated. Figure 1 shows that 4 element array structure on air supported substrate.Figure-2 expresses return loss of the proposed antenna designed. It shows that minimum S11 parameter is at 2.4GHz and another minimum at 2.9 GHz. So this will flexible for designer to choose any of the either point. Figure 3 shows that entire electric field (E) and magnetic field(H) distribution system in all direction.

Rectenna antenna circuit parameter analysis

Now, It is taken model structure and its equivalent circuit parameter in terms of Resistance, capacitance and inductance. The fresh diagram is taken where 50 ohm load and scattering parameter controller placed in a default frequency range shown which is shown in figure -4. To achieve suitable Simulation kind we have to place required component for SP as per figure. In figure 5, padded C & padded l are general capacitors and inductors .but this also give evidence to designers to enter desired spacing, width, and length of the element as per the element. That proposed structure to be used for actual PCB design.

CONCLUSION

From the above experiment we learned about to design a micro strip patch antenna in HFSS (High Frequency Structure Simulator). A 2.4 GHz rectifying antenna elements and its typical array structure is designed, which can adopt numerous power density if applied in different Rectenna array. The capacitance is exchanged by microstrip line in the form of dc pass filter and the diode in the rectifying circuit is joined in order. The energy translation efficiency from RF energy to DC electrical energy reached 80.25% by retaining 20.85 dBm and 3501 ohm resistive load through tedious testing correspondingly. So maximum 18.55 volt of DC output voltage is detected and noted during simulation. The entire circuit is designed and can be expandable to huge scale to produce mass electrical energy for any type of wireless power transmission.

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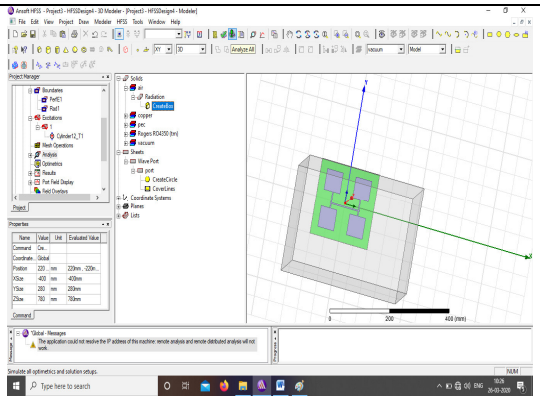


Figure-1(3D model design)

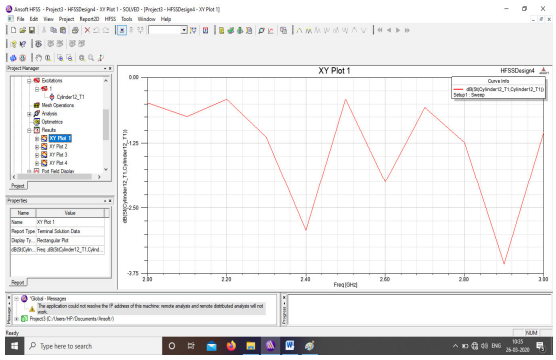


Figure-2(Return loss)

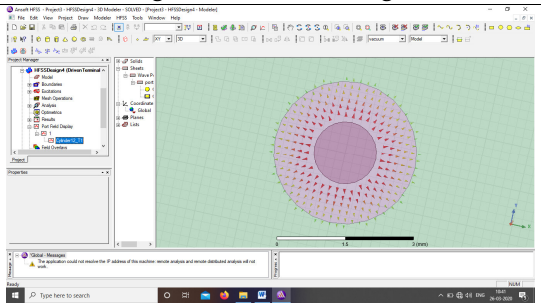


Figure-3 (E and H Port field disply)

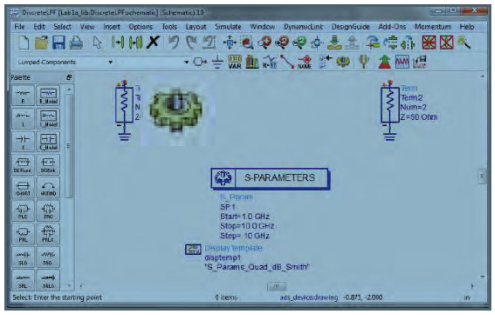


Figure -4 antenna circuit parameter

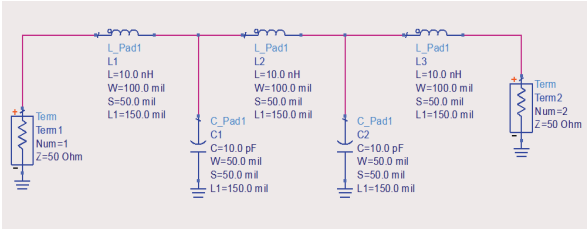
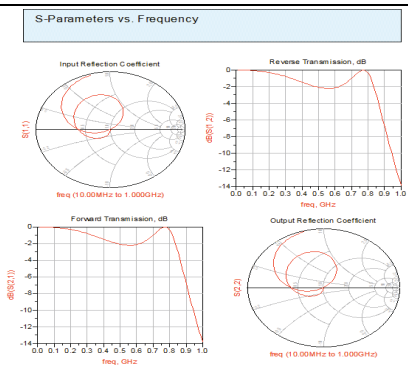


Figure -5 (lumped with element)



Now S parmeter verses frequeny is analysed and result is good.

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RESEARCH ARTICLE

Drive Test Analysis for a 3rd Generation of GSM System and its EMF Survey

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ABSTRACT

In this paper, Measurement, assessment is done for the coverage, capacity and quality of a mobile network. Then its result are measured and optimized. The technique involves of using a mechanical car holding mobile radio network air interface measurement kit that can detect and record a wide variety of the physical and virtual parameters of mobile cellular service in a given geographical area. Drive testing needs a movable transport system outfitted with drive testing measurement kit. The equipment are typically extremely dedicated electronic devices that interface to OEM mobile telephones. This confirms measurements are genuine and comparable to real user experiences. There are three requirement of drive test which can be termed as Network benchmarking, Optimization and troubleshooting, Service quality monitoring. For benchmarking, sophisticated multi-channel tools such as Focus Infocom's DMTS and XGMA, DingLi Communications' Pilot Fleet, Ascom's Symphony, Rohde & Schwarz-SwissQual's Diversity Benchmarker or Keysight Nemo Invex II are used to measure several network technologies and service types simultaneously to very high accuracy, to provide directly comparable information regarding competitive strengths and weaknesses. Results from benchmarking activities, such a comparative coverage analysis or comparative data network speed analysis, are frequently used in marketing campaigns. Drive testing to gather network bench-marking data is the only way mobile network operators can collect accurate competitive data on the true level of their own and their competitor's technical performance and quality levels. Similarly Optimization and troubleshooting diagnoses the root cause of specific, typically localized, network issues such as dropped calls or missing neighbor cell assignments and Service quality monitoring symbolizes the quality of service respectively.

Keywords: UWB system; parameter; time domain; bandwidth; Design; application

INTRODUCTION

This paper consist of 3G drive tests and EMF survey. It contains detailed method of the 3G drive test. It shows how use of the TEMS software for the 3G drive tests done. Drive test is conducted for testing coverage conditions of a cell site with RF drive test tool. The files collected by drive test tool as Log files are studied to evaluate various RF parameters of the network. And it's truly very vital things for mobile service provider. Drive testing help us to measuring and evaluating the coverage, Quality of Service and capacity of mobile system. TEMS Investigation is main tool of drive testing. It consists of both hardware and software. Hardware of TEMS Investigation is a mobile phone. The overall objectives of RF planning and drive test is to examine network health condition whose feedback is customer satisfaction in terms of coverage and capacity in real time.

3G DRIVE TEST

Site Information

Site information consists of site name, site id, latitude, longitude, mechanical tilt, electrical tilt. The drive test engineer is provided with these information before the drive test.

Drive Tools

First tool is a laptop with TEMS software which is an essential part of drive test. Second tool is a mobile with a TEMS license so that it can be detected by TEMS software. Third tool is the GPS (global positioning system) which detects the correct position.

Tools Setup Process

Open the TEMS software in the laptop**.**
Go to Presentation, then click GSM.
In GSM, click current channel shown in fig 3.

Tx Power – It is the transmitting power of the mobile station.
RSSI – It is Received Signal Strength Indicator. It is the total power of the entire common pilot channel received by the mobile station including noise and neighbor interference.
Target SIR – It is the target signal to interference ratio that mobile equipment is supposed to achieve by increasing or decrease its power.

SIR – Signal to interference noise ratio is the ratio of energy in dedicated physical control channel to that of the interference and noise received by the user equipment.
RRC State – It shows the current state i.e. idle or dedicated.
In WCDMA, click Serving/Active Set + Neighbors shown in fig 5.

Scrambling Codes (SC) – They are used to identify different cells of node B. There are two types of scrambling code i.e. primary and secondary scrambling code.
AS (Active Set) – It is the set of scrambling codes on which the user equipment is latched on and there can be at least three maximum scrambling codes in an active set.
MN – It is the neighbor cell detected by the user equipment.
In WCDMA, click Data services and then click HSDPA analysis shown in fig 6.
In WCDMA, click Signaling and then click Events shown in fig .7
In WCDMA, click Positioning and then click GPS shown in fig 8.
In WCDMA, click Positioning and then click map shown in fig 9.

Monitor the drive path through google map.
Then click on the 'Start Recording' and start the drive test.
Observe the parameters of the drive test shown in fig 11.

After the drive test is complete process the log file using TEMS software.
After the processing of log file, open Mapinfo. Professional software.
In Mapinfo. Professional software open the export file and generate the plot of required parameters.

- **Drive Plots**
- **Drive Route Plot**
- **RSCP Plot**

RSCP – It is received signal code power. It is the level of signal received by the user equipment or a specific common pilot channel received by user equipment.

Pilot Best Server Plot
Ec/No Plot

Ec/No – It is the ratio of energy of the chip and the combined power of all the signals including the specific pilot channel. It also shows the level of noise disrupting the specific CPICH.

HSDPA Throughput Plot

EMF SURVEY
Overview
The Effective Isotropic Radiated Power is measured by performing EMF survey across the BSS. Due to this survey, the harmful effect which causes due to huge power radiation can be checked from the tower. As per the customer's requirement, the different parameters are noted and report is prepared which will submitted to operator.

EMF survey tools: GPS, Digital camera, Laser distance meter, Magnetic Compass, Safety kit.

CONCLUSION

In this paper, 3G drive test is processed and each bit is covered. Different parameters are calculated and visualized to prepare a report of log File to reverse updating of GSM network. Here 3G RSCP Plot, pilot best sever plot and Ec/No Plot are improved.

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6. https://www.slideshare.net/SubhashKumar108/xcal-drive-test-tool

SSA	SITE NAME	SITE ID	LAT	LONG	SITE TYPE
BHU	K8 KALINGA NAGAR	BHU143	20.2793	85.7696	3G NEW

Fig 1 Site information

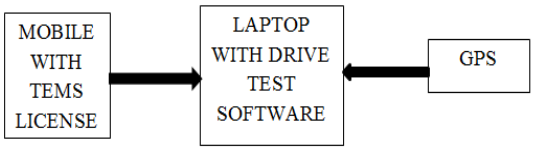

Fig.2(3G driving tools)

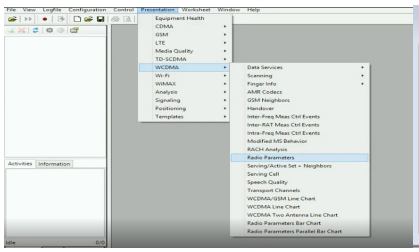

Fig .3 -TEMS Window

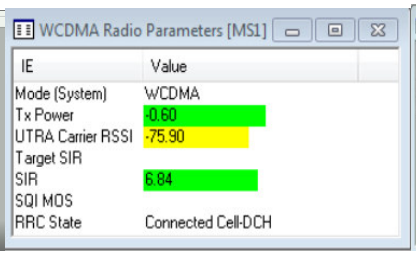

Fig .4 Radio parameters

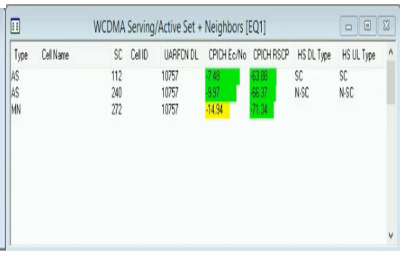

Fig.5.Serving /Active Set

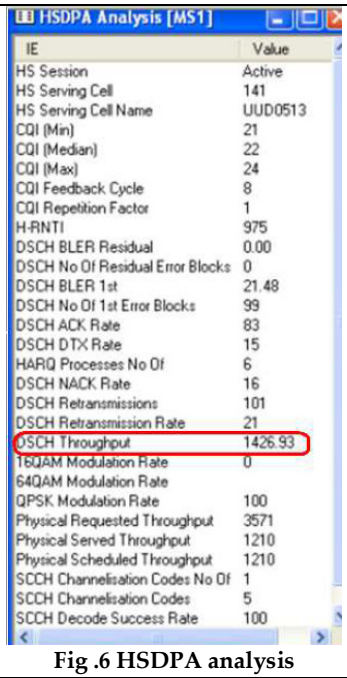

Fig .6 HSDPA analysis

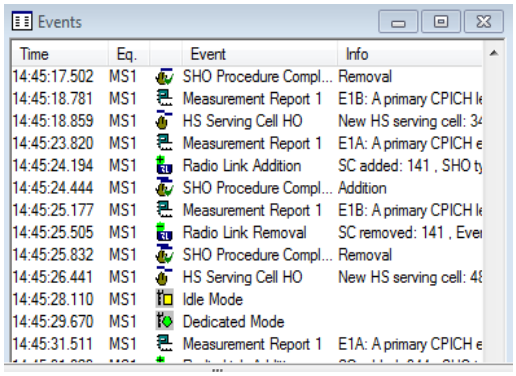

Fig.7 Events

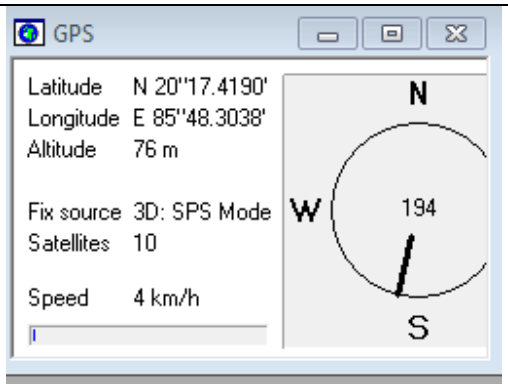

Fig .8 GPS

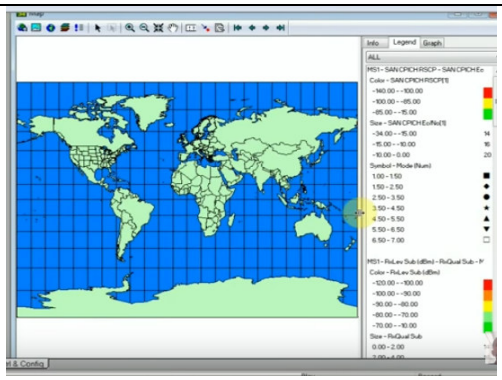

Fig .9 (Map)

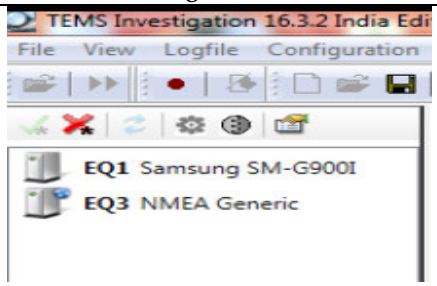

Fig .10 (Equipment Reading)

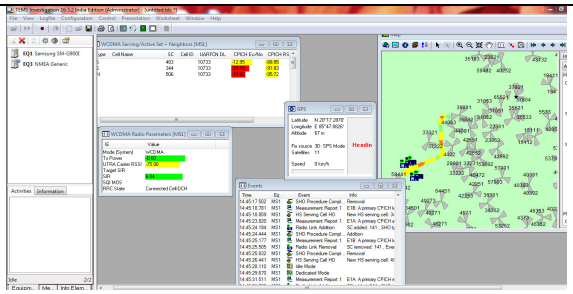

Fig .11 Tems window during 3g drive test

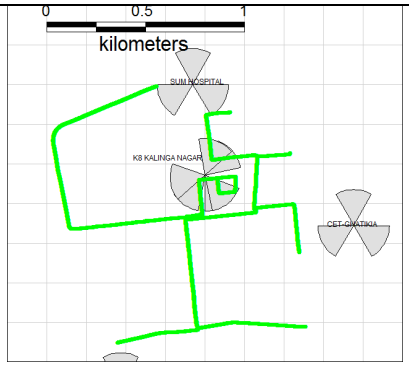

Fig .12(Drive route plot)

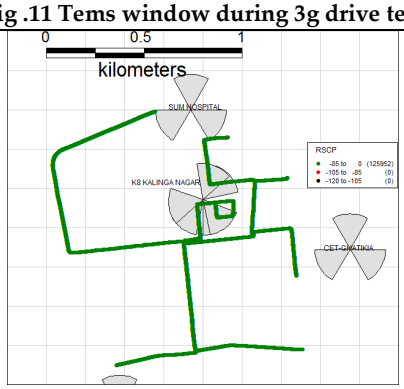

Fig .13(RSCP plot)

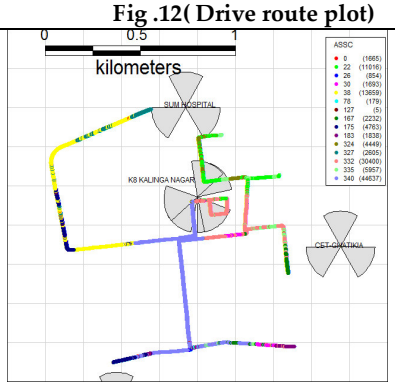

Fig .14 Pilot best server plot

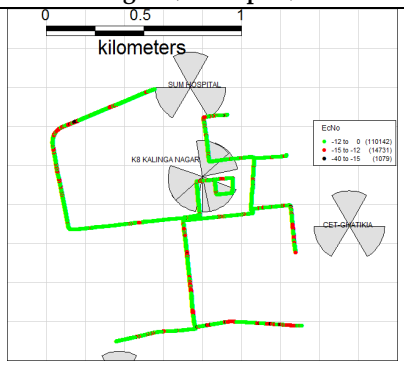

Fig .15 Ec/No plot

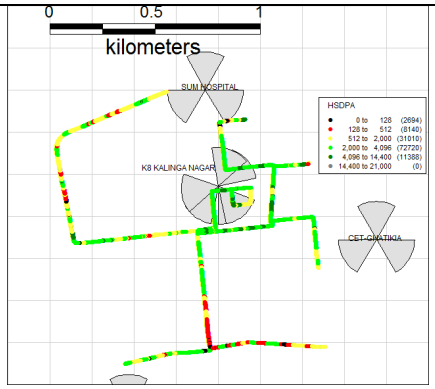

Fig .16 HSDPA throughput plot

Site Name :	RELIANCE FRESH
Site ID :	I-OR-BBSR-ENB-8123

Fig .17 Site information

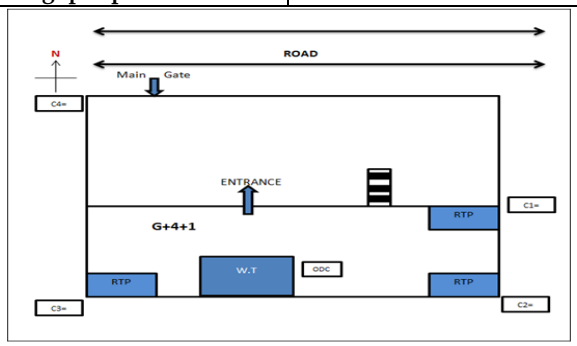

Fig .18 Site layout

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RESEARCH ARTICLE

Analysis and Report Generation of 4G LTE Drive Test: A Case Studies

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ABSTRACT

In this paper, Difference type of drive test summarized for 4G LTE Network and parameters such as Network benchmarking, Optimization and troubleshooting, Service quality monitoring. For benchmarking, sophisticated multi-channel tools such as Focus Infocom's DMTS and XGMA, DingLi Communications' Pilot Fleet, Ascom's Symphony, Rohde & Schwarz-SwissQual's Diversity Benchmarker or Keysight Nemo Invex II are used to measure several network technologies and service types simultaneously to very high accuracy, to provide directly comparable information regarding competitive strengths and weaknesses. Results from benchmarking activities, such a comparative coverage analysis or comparative data network speed analysis, are frequently used in marketing campaigns. Drive testing to gather network bench-marking data is the only way mobile network operators can collect accurate competitive data on the true level of their own and their competitor's technical performance and quality levels. For Optimization and troubleshooting Optimization and troubleshooting information is more typically used to aid in finding specific problems during the rollout phases of new networks or to observe specific problems reported by consumers during the operational phase of the network lifecycle. In this mode drive testing data is used to diagnose the root cause of specific, typically localized, network issues such as dropped calls or missing neighbor cell assignments. For Service quality monitoring, Service quality monitoring typically involves making test calls across the network to a fixed test unit to assess the relative quality of various services using Mean opinion score (MOS). Quality monitoring focuses on the end user experience of the service, and allows mobile network operators to react to what effectively subjective quality degradations by investigating the technical cause of the problem in time-correlated data collected during the drive test.

Keywords-UWB system; parameter; time domain; bandwidth; Design; application

INTRODUCTION

The paper includes 4G LTE drive tests. It includes detailed procedure of the 4g drive test. It contains the procedure of the 4g drive test and its parameters. It also includes the use of X-CAL software in 4G. Generally Drive test is conducted for checking coverage criteria of a cell site with RF drive test tool. The data collected by drive test tool as Log files are analyzed to evaluate various RF parameters of the network. And it's very important things for mobile service provider. Drive testing help us to measuring and assessing the Quality of Service, coverage and capacity of mobile network. TEMS Investigation is main tool of drive testing. It consists of both hardware and software. Hardware of TEMS Investigation is a mobile phone.

The overall objectives of any RF design depend on a number of factors that are determined by the needs and expectations of the customer and the resources made available to the customer. Analyses made through the information of data collected in the field represent a true picture of network conditions, and can be used in decision making in several areas, from planning and design through optimization and maintenance of the system, always with the goal of maximizing quality, capacity and coverage in the Network.

4G DRIVE TEST

Site Information

Site information consists of site name, site id, Band Type EARFCN. The drive test engineer is provided with these information before the drive test.

Drive Test procedure

The step by step procedure to perform drive test and collect required network parameter data is as follows:
Open XCAL tool on mobile so that the XCAL screen appears as shown below:
Press the setting button on the mobile and select FMS (Fleet Management System) mode.

After selecting FMS mode, there is need to select basic information i.e. band selection on which the network works, and the destination selection on which the drive test performs. Next, press select scenario; after pressing scenario five more fields are to be filled i.e. select SCFT from select type, enter site details for which drive test is performed, select Station 1 from test type (there are three stations and one by one test is perform for all the three stations), select count 1 from cycle option because the test is performed only one time, feed 55555 in dial number option and press save button. Next, press start button to begin SCFT test. A call is established in 55555 number. After 15 seconds the call is automatically disconnected and there appear queries to complete the test or the test is in progress, here option in progress is to be selected.

After pressing in progress the next station is to be selected till all the three stations are covered. After performing test (for station 1, station 2, and station 3) in place of in progress option, complete the test option is selected to complete the station test. Change test type from station1, 2, 3 to moving (the moving test is performed to test the internet speed). Next, select scenario; there are two parameters in select scenario option i.e., DTDL and DTUL. The moving test is performed for both DTDL and DTUL one by one. First the moving test is performed for DTDL, select DTDL from the select scenario option. Next, click to FTP to select the nearest server to perform moving test. Next, press start button to perform moving test for DTDL; in DTDL scenario XCAL tool downloads a video file from the selected server and calculate the downloading speed (maximum, average and minimum). By pressing the Auto call view the downloading performance is checked and also the downloading speed as well as the download throughput graph. Once the file is downloaded from the selected server, the call is stopped automatically and again query appears to complete the test or the test is in progress; select in progress option to perform DTUL test. Next, change scenario from DTDL to DTUL to perform the Data Uplink; again the FTP server is selected, the video file uploads from XCAL

to FTP server and the uplink speed is checked. By pressing the Auto call view the uploading performance is checked and also the uploading speed as well as the upload throughput graph. After completion of the DTUL test, the complete option is selected to complete all the tests.

Drive Plots

- Drive Route Plot:
- Coverage Plot (Mobility Event):
- MAC Layer Throughput Download:
- MAC Layer Throughput Upload:
- RSRQ quality plot:
- SINR quality plot:
- MCS downlink plot:
- MCS uplink plot:

CONCLUSION

In this project, 4G drive test is done in various method and EMF survey is done to know the signal strength for a particular area. Especially XCAL software gives good performance in LTE network. The drive root plot shows here clear image of radiation spectrum. Coverage plot (mobility event), MAC layer throughput download, MAC layer throughput upload parameter measured accurately. RSRQ quality plot, SINR quality plot shows comparison of quality survey and result are summarized. Here is another advantage is that modulation down link and uplink plot is drawn to measure the modulation efficiency.

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4. https://www.youtube.com/watch?v=lVixxswfjp0
5. 5.https://www.slideshare.net/syedmhussain370/wcdma-tems-parameters-investigation-and-drive-testing
6. https://www.slideshare.net/SubhashKumar108/xcal-drive-test-tool

Site Name	I-OR-BBSR-ENB-0291
Band Type	1800
Cycle	1
EARFCN	1326
Sectors Available	α, β, γ

Fig 1 Site information

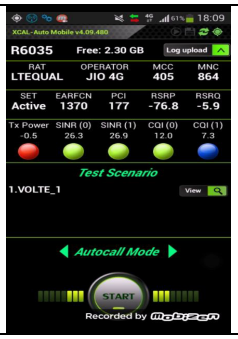


Fig .2 XCAL window

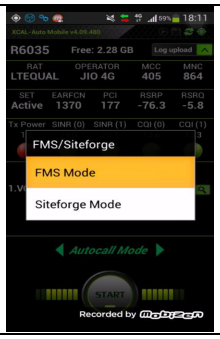


Fig .3 Selecting FMS mode

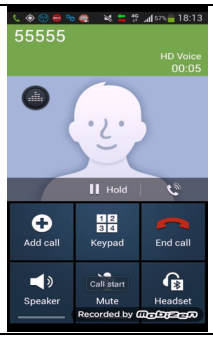


Fig .4 Call established

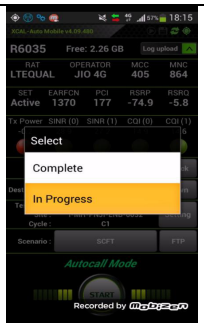


Fig .5 Selecting in progress option

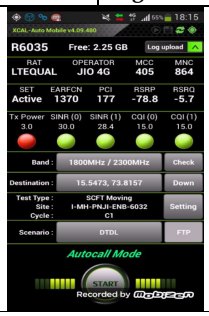


Fig .6 Selecting scenario

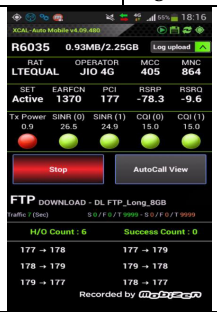


Fig .7 XCAL window during 4g drive test

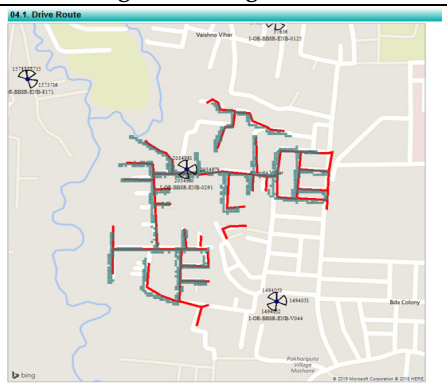


Fig .8 Drive route plot

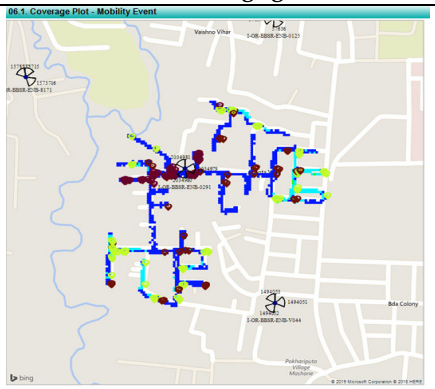
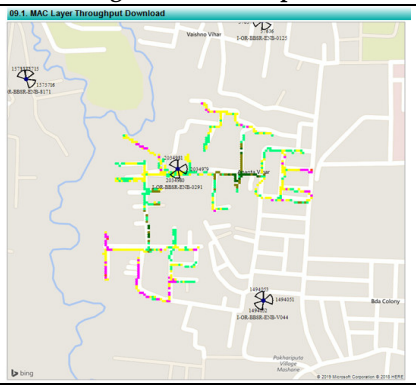


Fig .9 Coverage plot



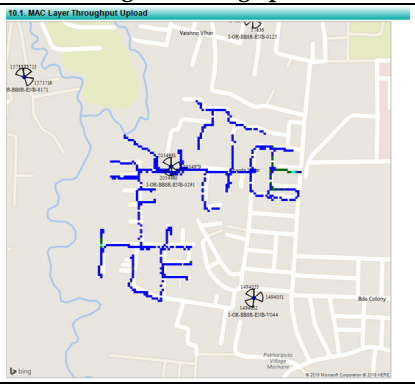
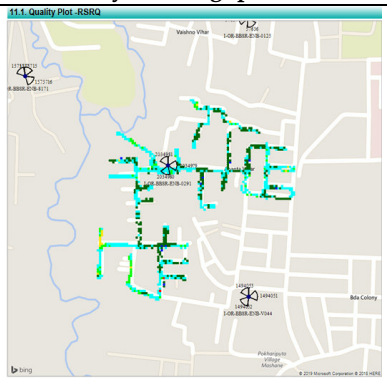
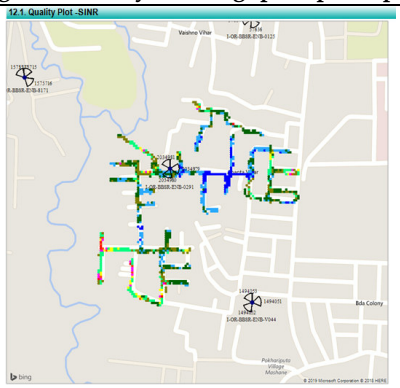
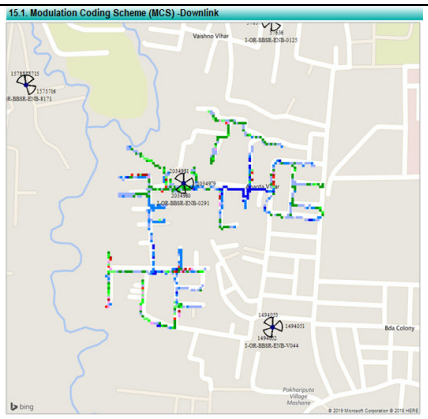
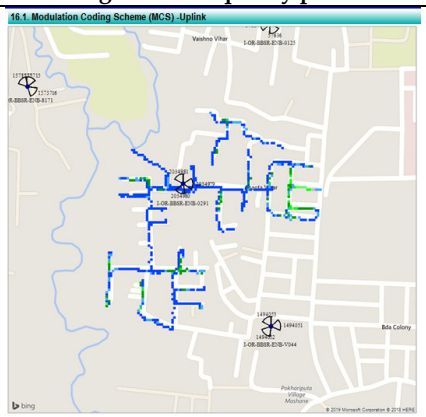


Fig .10 MAC layer throughput download plot	Fig .11 MAC layer throughput upload plot
 Fig .12 RSRQ quality plot	 Fig .13 SINR quality plot
 Fig .14 MCS downlink plot	 Fig .15 MCS uplink plot

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RESEARCH ARTICLE

A Case Analysis of EMF Survey and 2nd Generation Drive Test for a Telecommunication Network

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ABSTRACT

Abstract-In this context, Drive testing, its different types are analyzed, results are measured and optimized. Drive testing is a method of measuring and assessing the coverage, capacity and quality of a mobile radio network. The technique consists of using a motor vehicle containing mobile radio network air interface measurement equipment that can detect and record a wide variety of the physical and virtual parameters of mobile cellular service in a given geographical area. Drive testing requires a mobile vehicle outfitted with drive testing measurement equipment. The equipment are usually highly specialized electronic devices that interface to OEM mobile handsets. This ensures measurements are realistic and comparable to actual user experiences. Drive testing can broadly be categorized into three distinct topics named as Network benchmarking, Optimization and troubleshooting, Service quality monitoring.

Keywords: UWB system; parameter; time domain; bandwidth; Design; application

INTRODUCTION

The paper includes 2G drive tests and EMF survey. It includes detailed procedure of the 2G drive test. It shows how we use the TEMS software for the 2G drive tests. Drive test is conducted for checking coverage criteria of a cell site with RF drive test tool. The data collected by drive test tool as Log files are analyzed to evaluate various RF parameters of the network. And it's very important things for mobile service provider. Drive testing help us to measuring and assessing the Quality of Service, coverage and capacity of mobile network. TEMS Investigation is main tool of drive testing. It consists of both hardware and software. Hardware of TEMS Investigation is a mobile phone.

The overall objectives of any RF design depend on a number of factors that are determined by the needs and expectations of the customer and the resources made available to the customer. Analyses made through the information of data collected in the field represent a true picture of network conditions, and can be used in decision making in several areas, from planning and design through optimization and maintenance of the system, always with the goal of maximizing quality, capacity and coverage in the Network.

2G DRIVE TEST

Site Information

Site information consists of site name, site id, latitude, longitude, mechanical tilt, electrical tilt. The drive test engineer is provided with these information before the drive test.

Drive Tools:

First tool is a laptop with TEMS software which is an essential part of drive test. Second tool is a mobile with a TEMS license so that it can be detected by TEMS software. Third tool is the GPS (global positioning system) which detects the correct position.

- **Tools Setup Process:**

Open the TEMS software in the laptop**.**
Go to Presentation, then click GSM.

In GSM, click current channel shown in fig 3.
Time – It is the system time of computer.
Cell name – It displays the name of sector which is serving according to the cell file loaded in the TEMS software.
CGI – It stands for Cell Global Identity which is unique for every sector of the site. It consists of MCC (mobile country code), MNC (mobile network code), LAC (location area code), CI (cell identity).
Cell GPRS Support – It tells sector having GPRS or not.

Band – It tells in which frequency band the mobile is operating.
BCCH ARFCN – It tells by which BCCH is the mobile station getting served.
TCH ARFCN – It tells on which traffic frequency call is going on.
BSIC – It is base station identity code. It is a combination of NCC (network color code) and BCC (base station color code).
Mode – It shows in which state mobile is operating i.e. idle, dedicated & packet.
Channel Type – It shows in which channel the mobile is working.

In GSM, click radio parameters shown in fig 4.
Rx Level – It is the receiving level of the mobile from the site in terms of dBm.
Rx Quality – It is the quality of voice which is measured on basis of BER.
FER – It is Frame Erasure Rate. It represents the percentage of frames being dropped due to high number of non-corrected bit errors in the frame.

In Presentation, click Signaling, then click Events shown in fig 5.
In Presentation, click Positioning, then click GPS shown in fig 6.
In Presentation, click Positioning, then click Map shown in fig 7.
Connect the mobile and gps with the laptop and activate them.
Monitor the drive path through google map.
Then click on the 'Start Recording' and start the drive test.
Observe the parameters of the drive test shown in fig 9.

After the processing of log file, open Mapinfo. Professional software.
In Mapinfo. Professional software open the export file and generate the plot of required parameters.

(a) **Drive Plots**
(b) **Drive Route Plot**
(c) **Rx Level Plot:**
(d) **Rx Quality Plot**

EMF SURVEY

Overview

EMF survey is performed to collect EIRP (Effective Isotropic Radiated Power) ratio to know about the strength of EMF signal across the BSS. This survey is performed to check the harmful effect cause due to high power radiation of the EMF from the tower. Take data of the site i.e. site name, site id, site address, latitude & longitude. Take the tools required for the survey. After the survey the report is made according to the requirement of customers.

EMF survey tools: GPS, Digital camera, Laser distance meter, Magnetic Compass, Safety kit.

EMF survey snaps

Datas collected in EMF survey

Site layout, panoramic photos at 0°, 30°, 60° ……330° respectively, tower height, building height, tower photo, building photo, latitude & longitude of site, GPS photo, antenna height, azimuth, antenna snaps, tower base snap, corner snaps, adjacent building snaps(within 60 meters), adjacent buildings height, number of floors, latitude, longitude & distance, adjacent buildings layout, signage snap.

CONCLUSION

In this article, the detailed procedure of the 2G drive test is learned. Also learn about EMF survey procedures learned. Different parameters of 2G is also learned. Procedure of log file processing in TEMS software is taken and noted. I acquire skill in report making of drive test and EMF survey and learned about different types of reports. It is gained a lot of experience in the field of drive test engineer. Also this is gained some knowledge about the working of mobile towers practically.

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3. https://en.wikipedia.org/wiki/Drive_testing
4. https://www.youtube.com/watch?v=lVixxswfjp0
5. 5.https://www.slideshare.net/syedmhussain370/wcdma-tems-parameters-investigation-and-drive-testing
6. https://www.slideshare.net/SubhashKumar108/xcal-drive-test-tool

SSA	SITE NAME	SITE ID	AZIMUTH	LAT	LONG	MT	ET	MODE
BHUBANESWAR	RICHIREGENCYVIM_SRAN	ORBHU-311	60/160/245	20.29569	85.81661	1/2/1	0/2/0	2G

Fig 1 Site information

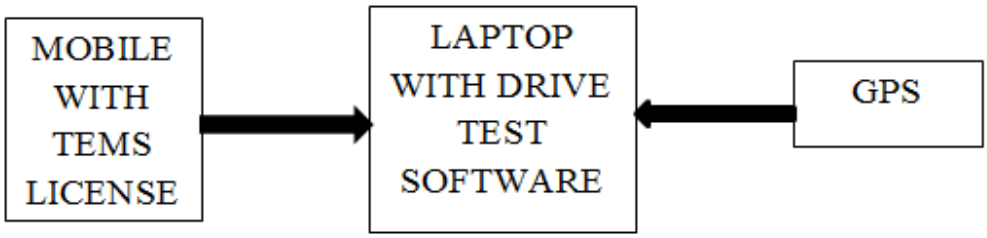

Fig.2.Drive Tools

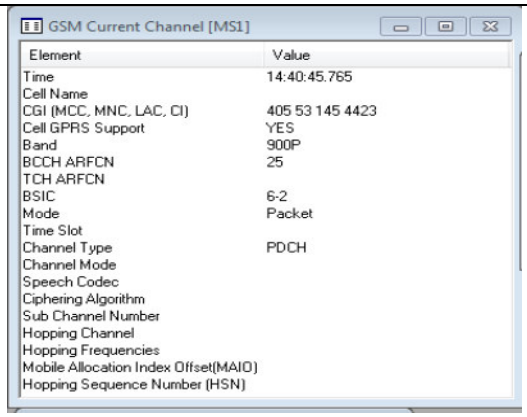

Fig .3 GSM current channel

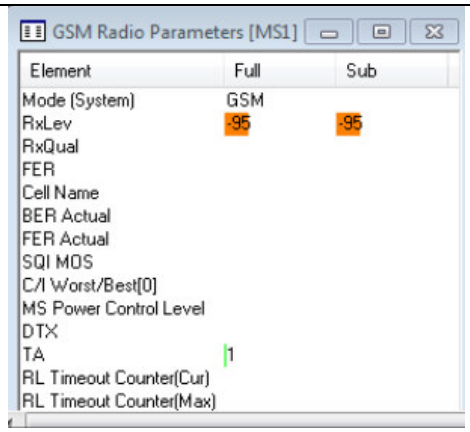

Fig .4 GSM radio parameters

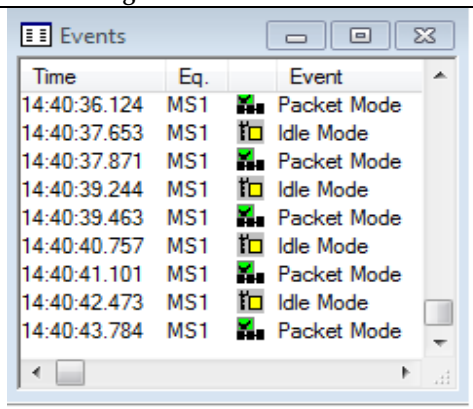

Fig .5 Events

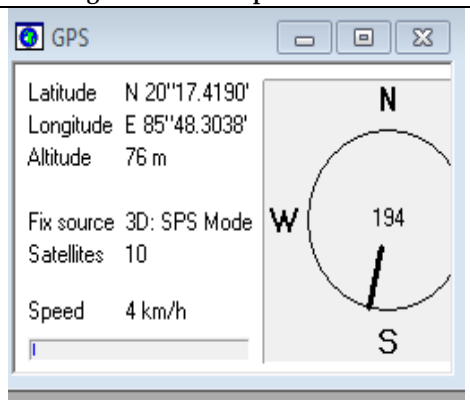

Fig .6 GPS

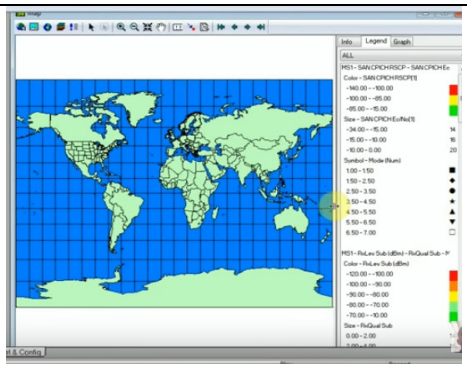

Fig.7 Map

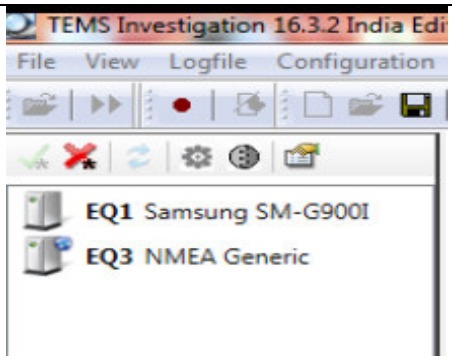

Fig.8 Equipment Reading)

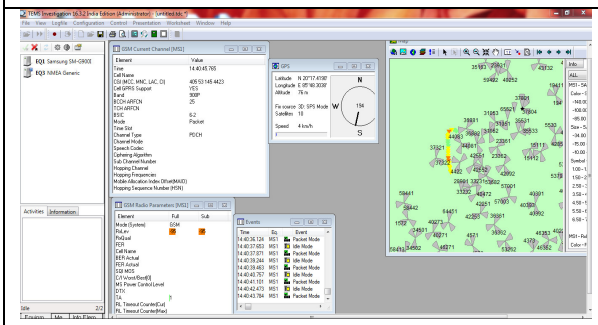

Fig .9 Tems window during 2g drive test

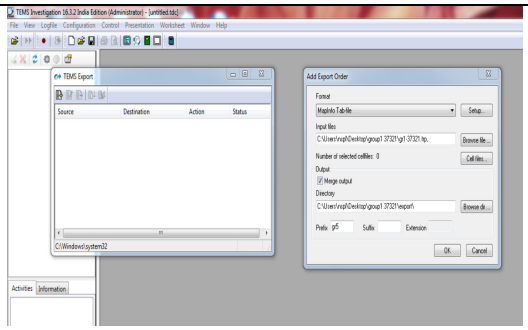

Fig .10Logfile processing window

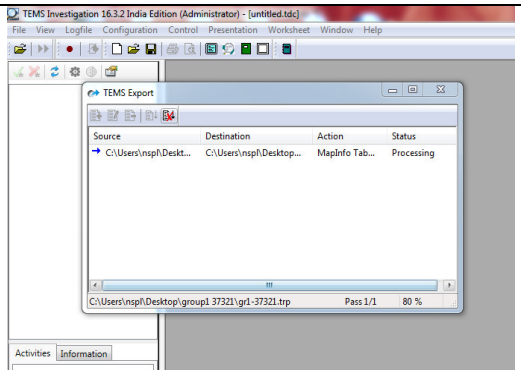

Fig .11 Log file processing

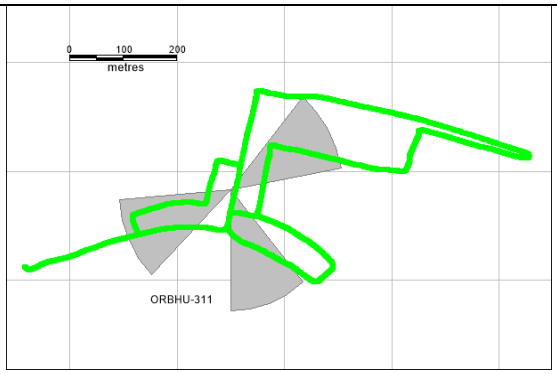

Fig.12 Drive Route Plot

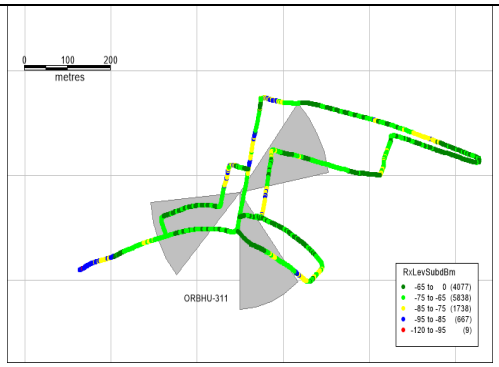

Fig.13 Rx Level Plot

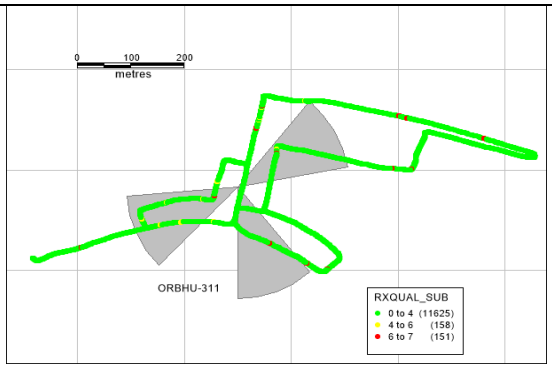

Fig .14 Rx quality plot

Site Name :	RELIANCE FRESH
Site ID :	I-OR-BBSR-ENB-8123

Fig .15 Site information

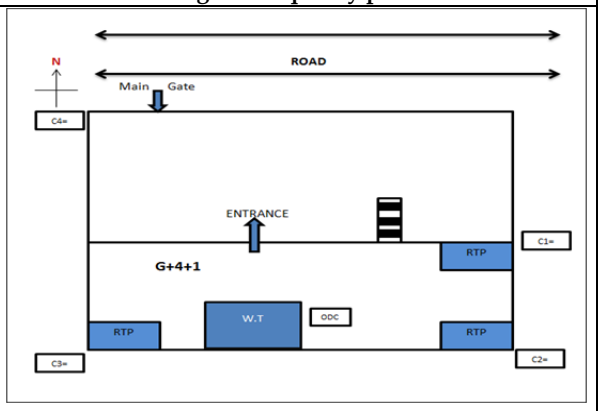

Fig.16 Site layout

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RESEARCH ARTICLE

A Study of Computer Graphic Image AnimationTechnique

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ABSTRACT

Recently, educational computer animation has turned out to be one of the most elegant tools for presenting multimedia materials for learners, and its significance in helping to understand and remember information has greatly increased since the advent of powerful graphics-oriented computers.In this paper we have presented a study of various graphic image animation techniques and their probable usage in educational learning.

Keywords: Computer graphics, animation,three dimentional motion data,educational learning, feature database

INTRODUCTION

Animation isn't simply the motion of few characters on screen however it's additionally a good medium to form folks perceive the message, particularly young children. Animation, which is basically a form of pictorial presentation, has become the most prominent feature of technology-based learning environments. It refers to simulated motion pictures showing movement of drawn objects. Looking at the past and the present, animation has evolved over time. It started with pieces of paper and rope in 1828 and is today three-dimentional animation videos.Recent years have seen enormous interest in research on two-dimensional image manipulation.Very powerful solutions have been presented for issues like matting, image complementation, texture synthesis and rigid image handling.If images are manipulated, unavoidable requirements are tools to produce correct division or matt alpha and to complete lack of pictures.

Generating videos by animating objects in still images has countless applications across areas of interest including movie production, photography, and e-commerce. More precisely, image animation refers to the task of automatically synthesizing videos by combining the appearance extracted from a source image with motion patterns derived from a driving video.For instance, a face image of a certain person can be animated following the facial

expressions of another individual. In the literature, most methods tackle this problem by assuming strong priors on the object representation and resorting to computer graphics techniques.

Animation System

An artist faces two challenges when creating a two dimentional animated character to mimic a specific human performance. One is the artist must design and draw a collection of artwork depicting portions of the character in a suitable set of poses, for example thigh and leg poses that can be selected and combined to express the range of movement and muscle flexing typical for that person. Other one is in order to depict a specific performance, the artist must select and position the appropriate set of artwork at each moment of the animation.

Designing the motion of 2D or 3D characters is a critical part of creating animated stories. Relative to traditional keyframe-based workflows, performed animation provides a more convenient way to specify how characters move. Instead of authoring individual frames or specifying motion curves, an actor simply demonstrates the desired movements, which are acquired via video or motion capture and transferred to the character. For most three dimentional characters, the motion transfer is relatively straight forward. Each joint on the actor typically corresponds to a matching joint on the character, which allows the continuous motion of the performer to be mapped directly to the three dimentional character producing convincing, nuanced animations. As a result, performance animation is used for a wide range of three dimentional animation scenarios, from feature films to games to special effects.

Method I

To create convincing animations of a two-dimentional character, its shape has to be deformed in a plausible manner, while maintaining minimal effort to generate animations.The basic idea is to utilize a set of generic form templates T, representing the topological changes of a generalized model of character for a variety of camera viewpoints (Figure 1).The models are designed with a semi-automatic character approach.A model is known as a two nonmanifold dimensional triangle mesh that enables different animated layers to be represented.For example, for animation from a side view, for separately moving parts of the body we must consider different layers, for example one layer for the forearm, one for the body, the fore leg and another for the rest of the arms and leg.In addition, such layers can not move separately but must be "stitched," in order to convey a connected body impression when animated.Thus, a triangulate set of vertices representing the boundary form and skeleton joints for each layer of T template consists of.Each template's different layers are linked by common border vertices.Inside each layer, additional vertices are added, allowing us to make more realistic animations by "inflating" the shape templates before animation.To deform T we employ a form-handling technique as-rigid as-possible (ARAP), on the one hand allowing for flexible deformations of the shap of the character and on the other, preserving the body size and appearance ratios to bind the distortion on the character.

Method II

Measuring the three-dimentionalposition of points on surface of any complex object is a significant problem.Moving every point a small distance in successive frames is to shift the position of object from one to another.The location of each skin point is determined by the interpolation between the previous position of the stage and the next position of the process.By blocking a number of key drawings, the animator specifies the desired motion.He then gives the assistant animators the main drawings which generate the necessary intermediate frames (Figure 2). The key drawings are replaced by data files which describe the object for each of the various poses.As the motion is non linear, to estimate the acceleration and deceleration of facial movements, a cosine interpolation scheme can be used. Each frame has a phase number associated with it. This phase number is a real number whose integer part refers to the preceding phase and whose fractional part indicates the location of this step between the preceding and the next step.The following algorithm is used to measure every part of a Point position:

Current position = position in the previous phase +C * difference wheredifference = position in next phase - position in previous phase C =(1.0 – cos (Φ)) / 2.0and Φ = phase fraction * 3.14159

Animation Program Algorithm

Step 1: The animation program contains topology and phase data arrays.In the program up to three passes may be stored.In data files the topology and phase data are read in.The program user interacts with it to specify which data files it wishes to read in.
Step 2: Phased datafiles are data for a point set.Each point has a point number and a three-dimensional position.Topology data is a specification for every object poygon.The polygon specification consists of the polygon vertices and their color.
Step 3: After reading in the desired data, ither half of the object data is constructed by mirroring or reflecting data for the first half of the object.
Step 4: For each frame of a sequence, a number of tasks must be accomplished to calculate the data needed to pass to the hidden surface and shading algorithm.
Step 5: The software interpolates the phase data to obtain the location of each vertex in the skin for this structure using the phase number assigned to each container.
Step 6: These points are specified in a system centered in the coordinates.The surface hidden algorithm will require data in a separate coordinate system to be specified.We want to take a look into the position of the new coordinate system , known as the viewing system.The Z axis of the display system should show the direction that we want to look at. This new coordinate system must convey position data.The animation program translates the data so that the source moves from the center to the position from which we want to look.The coordination mechanism then rotates such that the Z-axis of the viewing mechanism points to the position we want to see.
Step 7: The usual to each polygon is determined after the data are transferred into the viewing device.The normal at each skin vertex is determined using these normals.For each vertex, this is achieved with the average of the rising standard polygons of the vertex.
Step 8: For each frame, following parameter are passed on to hidden surface and shading algorithm:

1. The Viewing angle
2. The color of each polygon
3. The position of beginning and ending point of each edge of each polygon and the normals at these points.
4. The desired resolution.

OBSERVATION AND CONCLUSION

Animated sequence can be recorded using animation camera. Film advance and shutter to be under program control. Designing educational materials with the aid of the mentioned technique, while considering the types of temperament of students, is a really promising avenue to improve the learning process. Teachers will be able to feel more confident in the presentation of their lessons, in addition, they will become more competitive and professional. An analysis ofthe system for animating two-dimentional images of arbitrary characters with three-dimentional motion has been presented. It has been shown here that the simple user interaction, namely the selection of some two-dimestable joints, can be used to automatically reconstruct a geometrically plausible calibration of the camera and model from motion data.Forms deformation algorithm, able to deform the form in a more accurate way so that a wide variety of characters from various three-dimention motion dates can be generated by still frames and animations.With this could integrate global effects like shadows or reflections to improve the visual appearance.This study also has a high probability of broad educational benefits.

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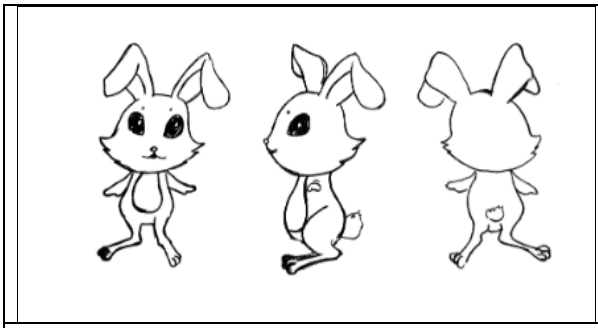

Figure1. Set of three shape templates generated by cycling in 90 degree steps around a character. (Frontal view, side view and rear view)

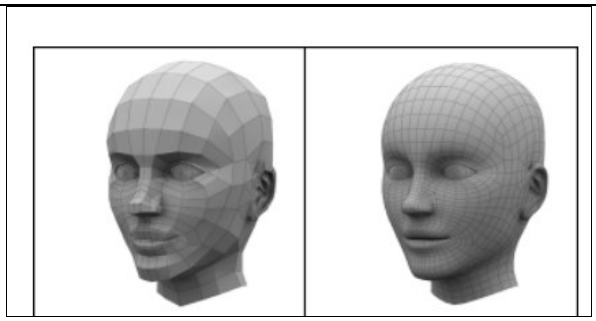

Figure 2. A polygon model before and after sub division

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RESEARCH ARTICLE

Design of a Microstrip Slot Antenna

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ABSTRACT

This paper describes simulation study of a printed microstrip slot antenna.It is a quarter wavelength monopole slot cut in the edge of the finite ground plane and fed by a microstrip transmission cable.It provides a broad impedance bandwidth customizable by variance of its parameters such as relative permittivity and substrate thickness, width and position of the slot in the ground plane, and measurements of the feed and ground plane.The ground plane is thin, 20 mm × 10 mm, around the size less than of a Laptop wireless card.At the center frequency of 5.5 GHz, its 50 mm width is about $\pi/2$ and significantly affects slot impedance and bandwidth.An impedance bandwidth of up to 70% (S11 = -10 dB) is achieved by individually optimizing parameters.

Keywords: Microstrip slot antenna, finite ground plane, microstrip feed line, monopole, wide band width.

INTRODUCTION

Merging wireless communications applications require challenging antenna features.Some of these applications include local multipoint fixed wideband communication services, while others address small mobile units such as cell phones or other handheld units, laptops and various remote sensing devices.Most technologies need miniaturization.The need to increase information transfer also requires bandwidth enhancement, without sacrificing performance.These requirements, put together, provide a challenging list of specifications requiring antenna design innovation beyond known conventional techniques [1-2].Miniaturization of antenna for mobile phones, PC cards and wireless personal digital assistants (PDAs) is also of interest[3].A slot antenna is important for such applications because of its simple structure.If a microstrip slot antenna is fed with a microstrip thread, it does not add weight and size to the device and is appropriate for these applications [1-3].Consequently, much attention has been paid in the past to analyzing narrow-width rectangular microstrip slot antennas fed using a microstrip line [1],[4],[5].The authors presented the design of printed square slot antennas fed by a microstrip line with a fork-like tuning stub to enhance bandwidth.Simulation results for low-profile, wide-band quarter wavelength microstrip monopole slot

antennas fed on a finite ground plane are shown in [7-8]. A diversity antenna with two feed ports was recorded using a monopoly and socket, where a quarter wavelength channel antenna is combined with a quarter wavelength monopoly [9].

In this paper, we present simulation and experimental traces of a printed microstrip slot antenna fed by a microstrip line.The antenna is a quarter wavelength monopole slot, cut in the edge of the finite ground plane and fed by a microstrip transmission line.Because the ground plane is rectangular, two different slot locations are possible along the long and shorter edges of the ground plane.For the former case, Section II examines the problem in detail. It has different design parameters for optimization.The effect of individual slot performance parameters is investigated.These investigations provided adequate information to understand slot antenna characteristics on a small, finite ground plane.Therefore, to have polarization flexibility, the second orthogonal slot case was not analyzed in depth, but instead in tandem with the first.Section III presents the results. These slot antennas can be easily integrated with planar circuits and electronics using their ground plane conductor.The simulations were performed using a "High Frequency Structure Simulator" HFSS 17.0 finite element system (FEM) software.

GEOMETRY AND PARAMETRIC STUDY

The antenna is a straight slot cut on the ground, as shown in Fig. 1and fed a 50 microstrip transmission line electromagnetically.Table 1, which has been selected after many simulations, provides its initial design parameters.Its length is 7.2 mm Sl and its design frequency at 5.5 GHz is a quarter-free wavelength.And it is a slot antenna of the monopoly.For the parametric study the most sensitive parameters were Sw, Sp, Gw and Fl. Fig.2. Microstrip slot antenna design using HFSS The remaining parameters showed no significant impact on impedance bandwidth and were kept invariant throughout.For a correct understanding, only one parameter at a time was different, while others were maintained constantly.This reduces the operating frequency by increasing the slot width, which increases the slot zone.Therefore, this parameter can be used to reduce the slot size relative to the wavelength.The minimum frequency S11 is not Gw-sensitive.Once again, the best impedance match frequency is reduced by increasing the relative dielectric constant, which can be used for slot size reduction. The impedance bandwidth can be increased by varying the substrate thickness. The best frequency matching impedance remains practically constant with increasing feedline length. Thus, the feedline length variation modifies its impedance transformation ratio and compensates the slot impedance variation with frequency, increasing its bandwidth.

The parametric analysis above showed the effect and action of each parameter on the bandwidth of the antenna impedance.The results can be useful in selecting optimum variable parameters when certain others are constant due to design and manufacturing constraints.Due to multiple parameters, however, individually optimized parameters will not result in optimum antenna design.On the other hand, as all optimized cases provided peak bandwidths between 35–40%, the selection of individually optimized parameters for a prototype antenna should do the same or better.The antenna impedance's sensitivity to substrate height is a practical concern and was investigated for the above antenna.Increasing the substrate thickness actually increased the bandwidth. The increased substrate height basically increases the slot antenna 's electrical dimensions, which in turn provides increased bandwidth.At the lowest frequency of 5.5 GHz, this range is about a quarter wavelength and around.Hence, its variable impedance transformation is much more efficient and further improves slot impedance bandwidth.This feedline impedance transformation appears to be the most effective bandwidth parameter.

Simulations Results

The return loss, radiation patterns, 3D plot of the single slot antenna have been simulated.However, due to their asymmetric locations on the ground plane when dual slots are there, their radiation patterns are not exactly

similar.This can be corrected or improved in practice by selecting alternative and symmetric locations, depending on the substrate circuit configuration.

CONCLUSION

Printed microstrip slot antennas were investigated in this article, showing variable and large impedance bandwidths, achievable by varying the specific parameters.This antenna can find wireless communication applications where simple wideband and compact polarization diversity antennas are desired.A microstrip slot antenna was also studied and showedwide impedance bandwidths and potential for polarization diversity applications.

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Table1. Initial Design Parameters of Microstrip Slot Antenna

Antenna Parameters	Values
Slot length S_l	7.2 mm
Slot width S_w	0.4 mm
Microstrip feeding spacing L_f	3.059 mm
Microstrip feeding impedance Z_f	50 Ω
Microstrip feeding length F_l	15 mm
Coaxial probe impedance Z_p	50 Ω
Ground plane length G_l	20 mm
Ground plane width G_w	10 mm
Substrate material	FR4
Substrate material thickness h	1.6 mm

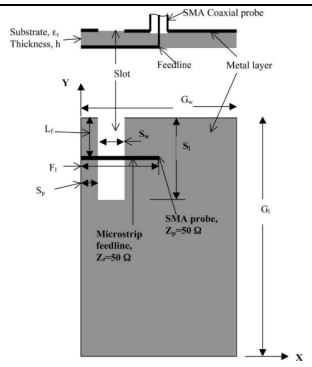

Fig. 1 Geometry and different parameters of a slot antenna

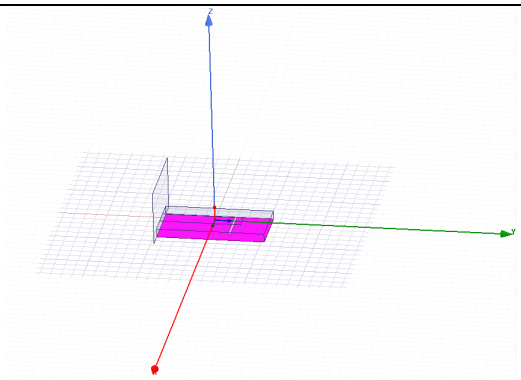

Fig.2. Microstrip slot antenna

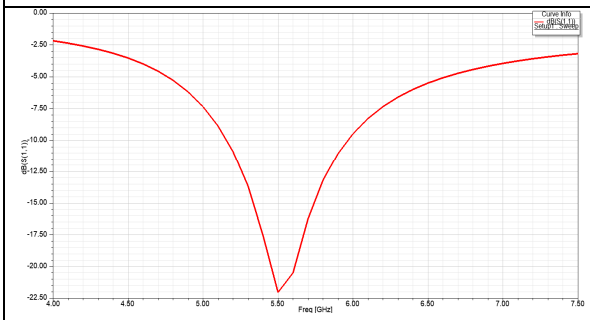

Figure 3. S_{11}plot of slot antenna

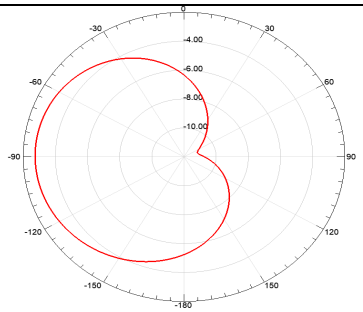

Fig. 4 Radiation Pattern at $\phi = 0^0$

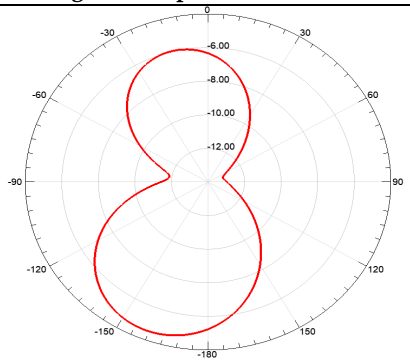

Fig 4. Radiation pattern at $\phi=90^0$.

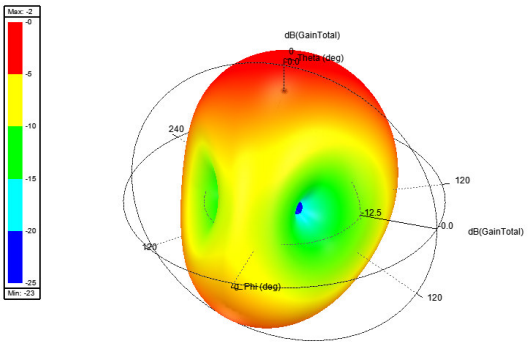

Fig. 5 3D polar plot of microstrip slot antenna

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RESEARCH ARTICLE

A Study of Microwave Filters

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ABSTRACT

This paper includes an analysis of the key techniques used in the construction of microwave filters.The foundation of much of a basic microwave-filter theory has been demonstrated in the field of lumped-element filters, in fact used directly for many applications at microwave frequencies up to 18 GHz.Many types of Microwave Filters are addressed, particularly for beginners to the field, with the objective of finding the most useful references.

Keywords: Bandpass, comb line, diplexers, filters, hairpin line, high-pass, low-pass, lumped element, microstrip, microwave, multiplexers, parallel coupled line, planar, strip line.

INTRODUCTION

Since the previous study reported in the 1984 Special Centennial Issue of this transaction [1], major changes have been identified.Since the previous study reported in the 1984 Special Centennial Issue of this transaction[1], major changes have been identified.Lumped-element filters are now used at a frequency of around 18 GHz and represent a significant percentage of the industry's generated microwave filters.The unloadable Q depends on frequency, but on average approximately 200, and can be obtained by values greater than 800 at lesser frequencies, e.g. 170 MHz[2].Such statistics favorably compare to the microstrip, and the cost of production is very small.Naturally, measurements are slightly smaller than distributed filters, a substantial benefit.The use of larger distributed filters cannot be avoided, however, unless installation failure and likely power supply are of significant concern.It is used technology.

The study of lumped-element filters is important academically as an essential part of understanding distributed filters, which largely rely on lumped-element theory.Therefore, a lumped element low-pass prototype filter begins to develop many or even most of the filter designs and the concepts of susceptibility slope and connection coefficients unify the theories (see Section III).Filters may be classified into several different categories and defined by the positioning of the insertion-loss-function poles and zeros in the passband in different classes of response

functions.The nulls are usually spaced throughout the passband for a rubbish or Chebyshev reaction, as the optimal reaction is far better than the flat or rare reaction of Butterworth.For poles, this type of filter response is the most frequent type at dc or infinity and is often described as a Chebyshev-all-pole filter or as a Chebyshev-filter simply.

When at finite frequencies one or more poles is incorporated into the channels, the filter is called a general Chebyshev filter or pseudo elliptical filter.The well-known elliptical function filter is the special case where the maximum number of poles are located at the end frequencies so that the stop bands have the same degradation level.This is rarely used because it has practical problems and is not ideal when specific stopbands are needed you rarely have to reject them until they are nevertheless frequent.The poles where they are most needed are nearly always better placed, as each additional finite frequency poles can increase complexity and expense.This discussion also covers the main filter categories defined by general reaction types such as low-pass, bandpass, high-passenger and band stops.For band stop filters, the poles are situated in the stop area and the zeros are positioned elsewhere, as normally created by means of a transformation of the low-pass band-to - band frequency stops.The topic of lumped element (LC) filters for service at microwave frequencies was fairly scarce in literature.This may seem surprising given the core role of LC filter theory, but textbooks do not go beyond the most basic stage of design, i.e. the application of low-pass transformations to band-passes.

The problem here is that when the narrow ribbon is set, the resulting filters become unrealizable due to the resulting large distribution of element values.Lose external coupling networks are required to transform impedances and implement impedance inverters and/or transform network work.The aim of this is to reach designs that usually have similar value for a mid-band reactance of 40 to 100, either in series or in a shunt or in numerous designs, series and shunt.This is the same state as the coaxial filter design, which indicates one of the few parallels between LC and tributed filter design.Some of these are described in the 1980s, the Microwave Journal published two papers [3] [4].Some of the design principles are shortly outlined, but for a more complete understanding many details are required.Either commercially available design programs are very lourd and require several arcane network transformation programs to produce feasible filters or lack the basic capacity.Interestingly, the fundamental 1957 paper by Cohn[5] gives one of the keys to a satisfactory design.

The paper describes LC filters with equal inductances and all-shunt resonators.This is, however, a little bit limited because all but one of the poles is at dc, and more general filters are needed as stated in [3] and [4].One way to do this is to position the required number of pole at dc and infinity using exact synthesis, which has the advantages of accuracy and no bandwidth limitations resulting from approximation.The best technique for synthesizing these methods is through the transformed variable that Orchard and Temes describe [6].Although this is not an easy subject, the techniques deserve to be acquired.Wenzel has provided a much simpler paper describing applications for the design of distributed filters [7], which must be studied first.[7] is almost similar with the techniques defined for LC filter syntheses, the distinction being that a simple transformation is initiallyused [1, Sec.].Moreover, [7] introduces the measurement line unit or cascading section required for distributed filters and which is not counter-part in LC filters. Exact synthesis also to best suit pseudo elliptical filters.One procedure is to synthesize a low-pass prototype, then a band-pass filter resonates.Network transformers are used to connect to, for example, serial condensers, as well as to introduce redundant LC-Element shunt when needed to remove "floating nodes." In some cases, the band pass filter can be synthesized directly without the low-pass prototype stage, such as when the poles are asymmetrically related to the passband, e.g. when thermocouples are asymmetrical. Further discussion is presented in Section III, with a particular reference to cascading-quadruplete filters (CQ) and cascaded-trisection (CT) filters [10], [11],[39], and this may be the basis for cross-connection filters between non-adjacent resonator filters.

UNLOADED QinMICROWAVEin LUMPED-ELEMENT RESONATORS

Returning to the issue of unloaded Q, the definition of that for the series LC resonator shown in Fig. 1. Isinstructive to consider.The resonator loss is caused by the resistance R.If the current in the resonant frequency is I, the value of the unloaded Q is defined as the ratio of the inductor reactance to series resistance, i.e.

$$Q = \frac{\omega L}{R} = \frac{\omega \frac{1}{2} LI^2}{\frac{1}{2} RI^2} \quad (1)$$

Similar results apply to a shunt resonator.In either case (series and shunt), the energies contained in the magnetic and electric fields are equal at resonance.We note that (1) for any resonator form, whether lumped or distributed, the concept of unloaded Q is precisely that.In fact, it is not even necessary to distinguish between the two since the Q of an LC resonator is determined primarily by that of the inductor and its Q depends on the ratio of its volume to surface area as in any electromagnetic resonator of the cavity.It has been established that a relationship of the form gives the Q of any normal (non-superconductive) metallic RF cavity.

$$Q = Kb\sqrt{f} \quad (2)$$

where b is a linear dimension of the cavity, fis the resonant frequency, and *K*is usually constant for any given type of resonator. It is noteworthy that a number of TEM resonators differ within a relatively narrow range, including lumped components, microstrip, strip line, and coaxial lines.It is normal in the U.S. to use units of inches for and gigahertz for f, and is then of order 1500–3600 for the different cavities, described differently as the mean diameter of the coil for LC resonators, the thickness of the substratum for microstrip, the ground plane spacing for strip line, and the outer diameter of coaxial line.

These figures relate to practical Q values for copper or silver rather than the theoretical values that are almost impossible to realize due to surface imperfections, and a de-rating factor of 0.7 was incorporated into any theoretical calculations.In the case of waveguides, the relationship between Q and dimensions is more complex than the simple equation (2),al-though the Q retains the same type of proportionality between frequency and linear dimension.For a given volume, however, the effective value is much higher than for TEM resonator cases.Later, in Section III-A, the value of a comb line filter increases as the ground-level spacing increases to an appreciable fraction of a wavelength, enabling the propagation of waveguide modes, leading to higher Q than predicted from standard TEM-type resonators.HFSS microwave filter design and simulation results are shown in Fig. 2 and Fig. 3.

TYPES OF MICROWAVEFILTERSANDDESIGN INFORMATION

This section describes the various types of distributed filters, where the different types may be used, as well as the key sources of design knowledge.These categories are comb line, interdigital, parallel-coupled-line band pass, band stop, ring and patch filters, and stepped-impedance filters.Several implementing media include waveguide, dielectric resonators, coaxial lines, evanescent filters and various printed microstrip, strip line and suspended substrates.Acoustic filters are beginning to make inroads into the market for high-volume miniature filters, typically used in wireless telephones, and details about microwave acoustics are found in this paper.Superconducting filters also come into vogue when the ultimate in performance is required, i.e. exploiting the extremely high unloaded Q due to virtual elimination of resistive losses.In some cases, the references cited may not be the earliest invention, but a more convenient or simpler description.Distributed filter design theories are similar to those for LC filters and are based on either exact synthesis or narrow-band approximation.The latter is briefly summarized in [8, pp. 432–433].The important concepts here are the definition of the coupling coefficients between resonators and between the

source and load resistors and end resonators, as well as a shunt resonator's susceptance slope parameter, which can be of any type, lumped or distributed,i.e.

Susceptance slope parameter = $b = \frac{\omega}{2}\frac{dB}{d\omega}|_{\omega=\omega_0}$ (3)

Where*B* is the susceptance of the resonator, e.g., for a lumped resonator

$$B = \omega C - 1/\omega L \quad (4)$$

After applying condition $\omega_0 = \frac{1}{\sqrt{LC}}$ gives $b = \omega_0 C$ (5)

For a quarter-wave short-circuited transmission line of characteristic admittance and electrical length

$$Y = B\tan\theta$$

$$b = Y\frac{\theta_0}{2} = Y\frac{\pi}{4} \quad (6)$$

Narrow-band filter designs for simple Chebyshev response are performed by forming the appropriate parameter of the susceptibility slope, and then replacing the formulas given in [8].Filters made up of resonators from the series are less common.They are merely the dual case of the shunt, and are also treated in [8].In the case of pseudo-elliptic filters, designs may be performed by deriving an appropriate low-pass prototype, followed by a low-pass transformation to bandpass (or band stop, or high-pass) and applying the same method of susceptance slope.Typically, a shunt LC "tank" circuit connected in series produces the finite frequency poles.In some cases, this can be done directly, obviously in the case of lumped filters, and by using a coupling condenser in the case of a comb line resonator, e.g., as in [9].However, by transforming the circuit into one that requires cross-coupling between non-adjacent resonators, as stated in [10], [11] and [39], it is more common to produce finite frequency poles.

Combline Filters

These are the most common types of coaxial filters at least for frequencies below 10 GHz because capacitive resonator loading results in a useful cut in size compared to the ones based on a four-wave resonance.They consist of an array of parallel resonators at one end with a loading capacitor at the other end.The resonators are positioned to make the short circuits all on one side of the filter and the capacitors on the other side.Here, redundant unit elements are added at the input and output ports to give a realizable internal impedance standard, and network transformations are implemented to give the transformers self and mutual admittance, giving functional physical measurements.However, such transformers are now rarely used in industry as they are somewhat inconvenient mechanically, and also increase filter length.Direct tapping of end resonators is more common, as described, for example, in [13].The main problem with this form of coupling is that it is inappropriate when the point is close to the shorter end of the resonator, as with narrow bandwidths at high frequencies, as it is then difficult to control.

Then using some form of magnetic loop coupling, which can be modified externally, is a good alternative.Another often very useful external coupling technique is to use "same-sided transformers"[14], which look like extra resonators at each end of the filter, as shown in Fig. 4(b) but have an impedance transformer position and do not contribute to the filter's insertion-loss function.Compared to direct tapping, the filter is lengthened, but this may not always be a problem, especially at high frequencies where dimensions are small, giving a robust coupling technique.Such filters also have a wide tuning range, with no coupling adjustments and little bandwidth change [14].The asymmetry of the insertion loss on the low-frequency side, especially with large bandwidths, is a drawback to combined filters.Sometimes it is possible to introduce an attenuation pole on the low side of the passband, but this can be difficult with wide bandwidth filters due to dispersion effects-the cross-coupling capacity has a linear

frequency dependence and the couplings between resonators are large , making cross-coupling between non-adjacent resonators mechanically difficult.

Other distributed filter types may be preferred.When ground-plane spacing is an appreciable fraction of a mid-band wavelength, waveguide modes become the predominant type of coupling, and the filter can no longer be considered a mere TEM line structure, but rather an evanescent waveguide filter (see[15] and Section III-H of this paper).This type of filter is very good with unloaded Q and is widely used in the base stations of telecommunications, particularly in pseudo-elliptical with cross-cutting, for optimal answering functions.Here, the rejection of the simple Chebyshev combline filter has better symmetry compared to the combline filters of smaller ground-levelspacing[15] since propagating waveguide filters have steeper rejection on the lower side of the passband, the opposite of combline filters.The "transitional" filter[15] is somewhere between these two extremes.

Interdigital Filters

These consist of quarter-wavelength parallels or 90 parallel couplings, which alternate between short and open ends as seen in Fig 5. The two are parallel-couplings.The equivalent circuit is an electrically separated cascade of shunt-short stubs and the electric length of the line can be a complete 90 unlike full-flow filters.In practice, the lines are shorter, because the fringing capacities are unavoidable, and it is advantageous in some cases that lines are shortened to 60, in order to achieve smaller filters with broader upper refusal bands, which can be compared with the one obtained with flash filters [7].They have looser inter-resonator couplings compared with comblinefilters, i.e.,the gaps between resonatorbars may belarger and, hence, simpler to produceathighfrequencies and wide bandwidths where dimensions become quite small. Inter- digitalfilters have been designed for suchbroad band widths and highfrequenciesas8–18,20–28,and28–40GHz,withupto23 resonators. Note that, when very broad bandwidths are specified, it is then difficult in practice (but not in theory) toachieve a return loss of better than 15 dB or so (0.15-dB

Parallel-Coupled, Hairpin-Line, Patch, and RingFilters

The original type of parallel line filters as shown in the Fig. 6. They are mostly done in microtrips or sometimes strip lines with higher microwave frequencies, as excessive duration in low loss airline situations prevents their economic application.The different phase velocities between even and odd modes in combined lines regions need to be taken into account in microstrips.Several papers on this subject, but few seem to indicate simple and work-saving design procedures.The indexes of previous issues in this article are referred to as "microstrip filters," with one of the simpler procedures given in [17], and further discussion in [18] and [19]. An extraordinarily important advance in microwave filters since the 1984 survey [1] is the development of ceramic resonator filters of the two main types:

- Resonator ceramic or "puck" filters.
- Dielectric-resonator filters in TEM-mode coaxial cavity.

The initial form theory has actually been defined very early, for example in [27]; however, the implementation has been delayed for several years due to a lack of adequate dielectric sealants with good temperature stability.They had been established and were commonly available in the 1980s[28] in many establishments.First-type ceramic resonator filters have a very small loss and greatly reduce the size of traditional waveguide filters.They can be single or double mode [29], but recent preference is to use single mode designs, given better stability in temperature and a slightly improved performance.

Suspended Substrate Stripline (SSS)Designs

SSS was first described by Rooney and Underkoefler[31] and proved important for the design of comparatively low-loss, high-band filters and multiplexers.It is highly suited for designing low-and high-pass pseudo-elliptic filters.An

accurate description of the techniques can be found in[1], and maybe the only subsequent paper to be included in the field is[19].This is apart from the considerable work on micromachined filters that use SSS in the form of a very thin membrane, a topic that is covered elsewhere in this TRANSACTIONS.

WaveguideFilters

The fundamental paper in this article is the well-known 1957 Cohn[5] paper, which is suitable for rectangular narrow bandwidth filters.If broader filters are required, more precise theories should be used as described in [1].Usually, a high-pass filter in waveguide is better configured as a broadband bandpass filter where the upper stopband is above the ideal operating band and is sometimes almost non-existent.Overall, this results in a shorter and lower loss filter that relies on the waveguide's cut-off frequency.Reference[1] also describes dual-mode wave-guide filters widely used in satellites and some terrestrial systems.Triple-mode filters are mentioned, but over-specialized programs are typically too complex.The main problem is the difficulty of tuning and, like dual-mode filters, the inability to tune such filters over even a narrow tuning range.

Coaxial Low-PassFilters

The very same, lumped and distributed mixed theory given in [33], which ensures good filter efficiency throughout the whole operating strip, extending up to the off frequency, is a more satisfactory technique for the system.The same theory may apply in all medium filters, such as coaxial line, stripline, microstrip, SSS, coplanary waveguide. The following may be used.

Evanescent-ModeFilters

The assumption that coupling between the nearest neighboring lines can be ignored is common when designing complete or interdigital filters.In the case of configurations in which the distance of the ground plane at the midband frequency is greater than 300 and where bandwidth is less than 1.5 (condition for the most common width-filter), spacing cannot be regarded as TEM anymore. (These are three hundred and six hundreds of them represent one free-space wavelength at midband).

CONCLUSIONS

In general, the subject of filters and microwave filters in particular is large, and at least one textbook has been generated for more than 1000 pages[8].The purpose of this paper is hopefully to simplify the entry points for field newcomers and show how the theory can be unified.Substantial filtering fields, such as tunable filters and active filter features, have not been discussed here, which can be considered as specialist topics and much less basic.The study of lumped-element filters has been shown to be a sound basis for understanding microwave filters, but in doing so, it is necessary to overcome standard textbook presentations restrictions and delve more deeply into the literature.Another important aspect of filter theory relates to its use in the construction of various kinds of liability elements, such as directional couplers, power divisors and phase shifters, subjects discussed elsewhere.

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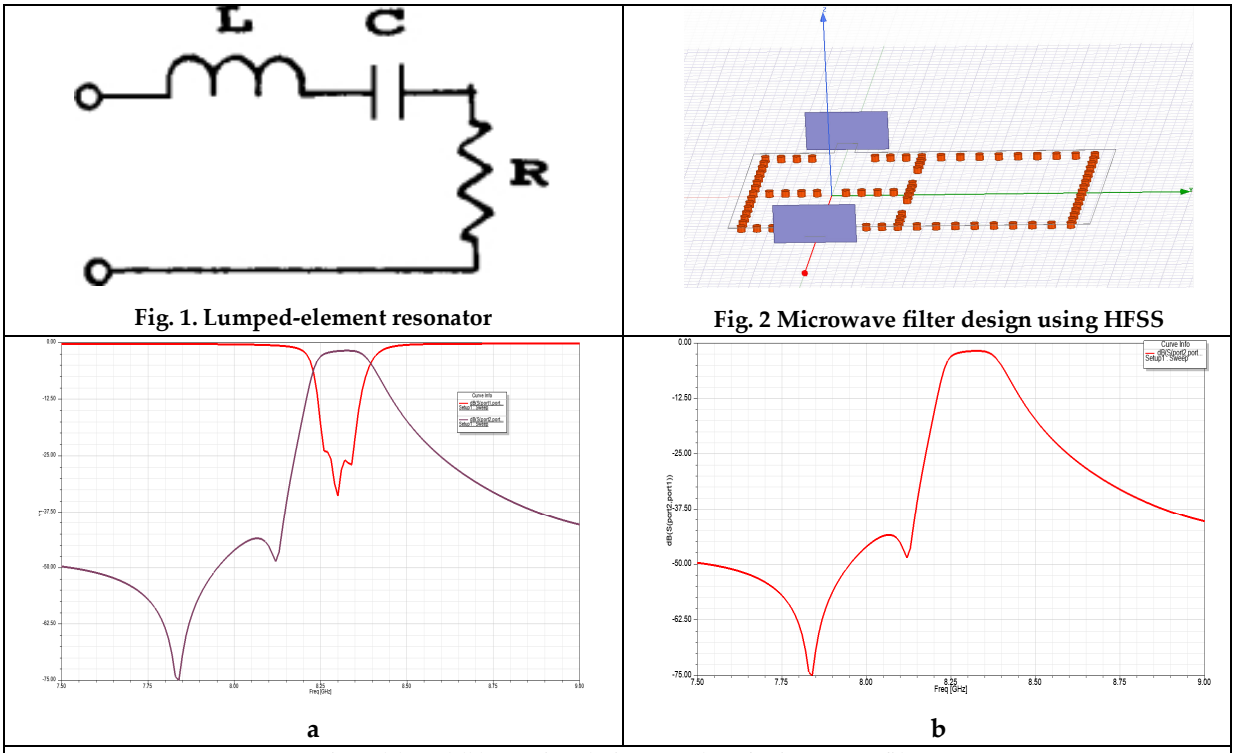


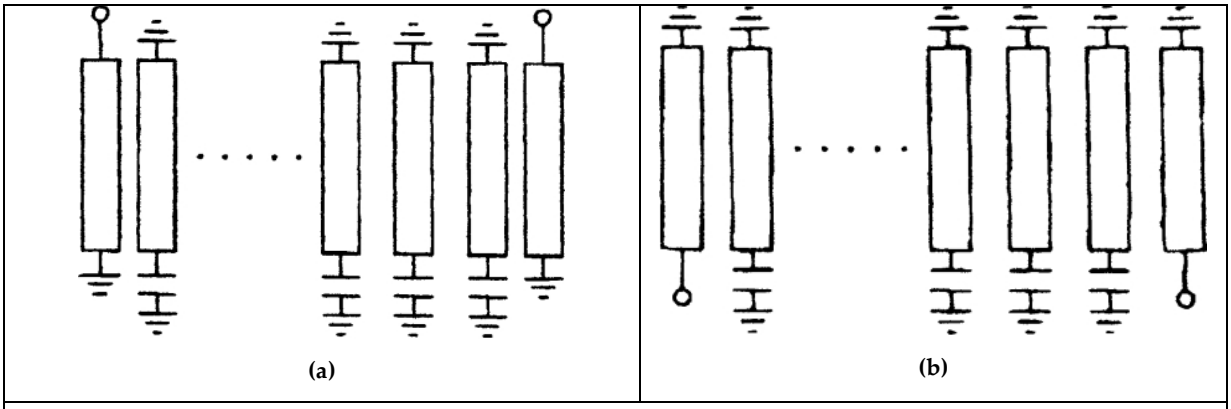
Fig. 1. Lumped-element resonator

Fig. 2 Microwave filter design using HFSS

a

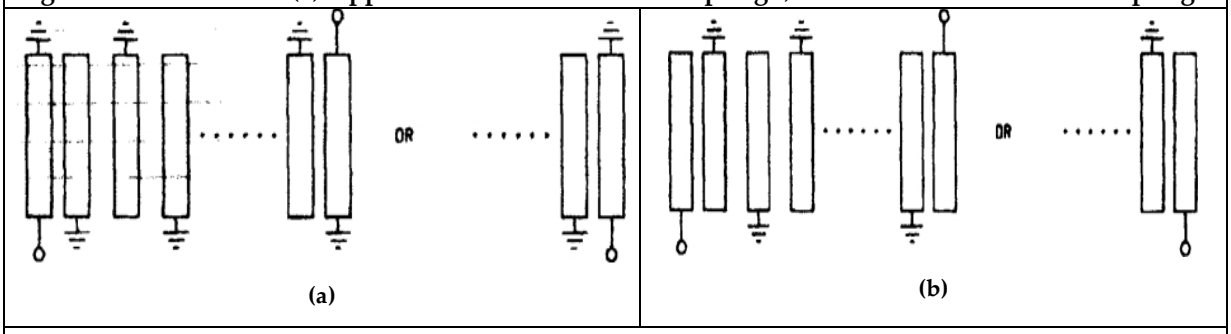
b

Fig. 3 (a) and (b) are simulation results of microwave filters



(a) (b)

Fig. 4. Combline filter. (a) Opposite-sided transformer couplingb) Same-sided transformer coupling.



(a) (b)

Fig. 5. Interdigital filter. (a) Short-circuited transformer coupling.(b) Open-circuited transformer coupling

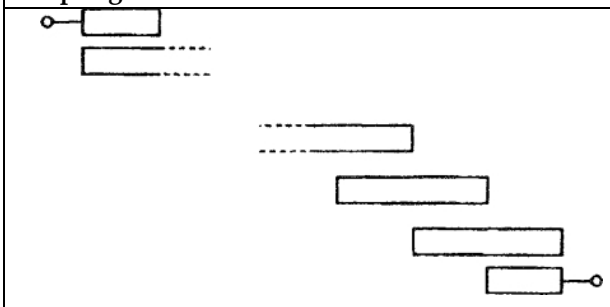


Fig. 6. Parallel-coupled-line bandpass filter.

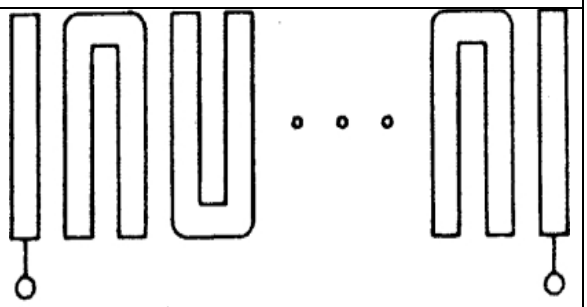


Fig. 7. Hairpin-line filter.

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RESEARCH ARTICLE

Multi-Level Security and Control System of Vehicle using Smart Technologies

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ABSTRACT

This paper is designed for the development of a multi-level security system to control the theft of a vehicle using GSM and biometrics. The main objective of this paper is to offer and advance security system in multiple levels to protect the car or any vehicle from unauthorized access using smart Technology. It provides real-time biometric user authentication to start the ignition. If the fingerprint does not match with that in the database, ARM produces the interrupt signal to initiate the alarm and also informs the car owner/authorized person about the unauthorized access via short message service (SMS) employingthe GSM modem. Further, GPS will be activated for tracking the action of the vehicle, at the same time the location-related information is sent to the user mobile phone.

Keywords: LPC2148, Fingerprint Sensor, Vehicle Security

INTRODUCTION

Automobiles are an asset in this ever-growing, fast-moving and insecure world. The fear of losing the asset in context has triggered the instinct of developing security systems to protect it from thievery. Many techniques have come forward to implement the security for the automobiles we dear so much. Researchers have used GPS modules implanted in their vehicles to enable the tracking feature. Even its used alongside a GSM module that sends the location of the vehicle on regular basis to inform the owner regarding the current location of the automobile. So the purpose of this article is to design a multi-level secured system to get rid of the anxiety of losing ones vehicle.

The purpose of this paper is to design a security model that would prevent the stealing of our vehicles. This article proposes the use of Biometric module to authenticate the access to vehicles, GPS module to continously track the

vehicle location, GSM module to intimate the vehicle owner the location. The proposed system utilises the above mentioned modules through a powerful and fast processor the "LPC2148" from the ARM 7 family. The processor is the heart and brain of the security module, it distinguishes the person accessing the vehicle is authorised or not. If not authorised necessary preventive steps are taken as programmed, else it continues normal sub-routines. Upon detection of unauthentic access it would start sending panic messages with location coordinates to the owner for tracking and recovering.

LITERATURE REVIEW

The foundation study reveals a number of proposed system that uses GSM and GPS based vehicle location and tracking system. The systems in question utilise the real-time tracking through the GPS satellites orbiting the Earth. The system uses geographic position and time information from the Global Positioning Satellites. Varieties of the anti-theft system have been proposed by different authors by using different technologies. This type of system consists of multilayer protection of the vehicle. The multilayer is as follows, 1) by using the fingerprint module [7], a key recognition system based on which doors are opened and closed, 2) Vibration sensors are used to protect the glasses, as soon as theft tries to break the glasses, it gives the buzz sound, 3) GPS tracker is installed in the car to track the exact location of the car and 4) GSM is used to send message to the owner of the car [4]. All the above four different technologies are interfaced with the ARM 7, which acts as a controlling unit [1][5]. In another literature survey, it has been found that they have incorporated the Biometric and RFID technology [2][6] for vehicle protection and authentication.

They have used a LabVIEW platform to test and validate the process [3]. Next-generation focus on IoT based security system by using Raspberry pi as the main Controlling unit and a WiFi [8]. The advantage of this type of system is that the car owner can seek surveillance from anywhere in the world. Another IoT based VAT is designed using Arduino and periodically the data is stored in the IoT cloud [10]. One survey found that there is a low-cost anti-theft system that uses only the mobile phone and no other devices [9]. The number of hardware I have gathered from previous journals and other sites is given below. All these are used together and worked according to our requirements.

PROPOSED METHODOLOGY

A multi-level control system of a vehicle includes a high level of security by restricting unauthorized users. It allows the user and makes him authorized whose fingerprint is enrolled in it. In case, any unauthorized user enters the vehicle, the Buzzer starts buzzing continuously and it uses GPS tracker to track the location of the vehicle and sends the whole information through GSM Module to the owner.

The flow of control starts from the top. Firstly, the user will be asked to place his finger. If the fingerprint matches the database enrolled into it then the vehicle door opens and if the fingerprint fails to match, the Buzzer starts buzzing and the GPS Tracker gets activated that sends the location of the unauthorized user continuously through GSM Module. Here, the Fingerprint sensor is connected to the LPC2148 ARM7 Board (using COM 0). GPS and GSM are interfaced with LPC2148 (using COM 1). LCD is interfaced with LPC2148 which is used for displaying purpose.The buzzer is connected to Pin0.23 and Relay Board is connected to Pin1.16 of the LPC2148.

Hardware & Software Description

The prototype model described in this paper focuses on many hardware and software parts. If we put together it forms the Embedded System. The embedded system comprises a main processing unit that has inbuilt memory to store code and peripheral devices like Fingerprint module, GPS Tracker, GSM Module, LCD to display information. Figure 3 shows the interfacing of LCD with an LP2148 ARM-based microcontroller. The LCD used in this model is 16 columns, 2 rows which can display 32 alphanumeric characters in two rows. Figure 4 shows the interfacing GPS

module with the main controlling unit with the help of the UART Port. UART port has two pins through which it sends and receives data.The system has an "onboard module that resides in the vehicle to be tracked and a "Base Station" that monitors data from the various vehicles.

The On-Board module consists of a GPS receiver, a GSM modem.Figure 5 shows the interfacing GSM with LPC2148 Microcontroller with the help of the TXD and RDX pin. These pins are universal serial communications pins through which data can be transferred from one device to another.The fingerprint module is interfaced and an application is used to new fingers of the users. This application may be useful for the enrolment and deletion of users. The SFG application for fingerprint enrolment is very simple to use. Finally, after the interfacing is successfully established the programmer need to go for the program implementation. We can see GPS, GSM, and fingerprint modules all are interfaced with the help of the UART protocol. The programmer has to use an IDE i.e. Integrated Development Environment which helps in editing, debugging, compiling the code. So the IDE used does the cross-compilation. It has an option to select the board which is to be used for prototyping development. For this model, we have used the LPC2148 development board, which has 2 input-output ports of 32 bit each. It has many features thatare supported by UART, SPI, I2C, USB 2.0, VIC, WDT, Timers/ Counters, Interrupts. So out of all the features listed above, used only UART and Interrupts to work with all the peripheral devices.

Hence Keil uVision 5 IDE is used to write the code. Once the code has been written and tested and made bug free, a hex file has been created using the IDE. There is another application used to upload the hex file into the target hardware. This application is known as Flash Magic. All the applications discussed above must be installed on the laptop or desktop and with a USB to UART cable the hex file is to be uploaded into the LPC2148 Microcontroller. Finally, in a single environment, we can test, verify, and optimize the application code. The whole prototype model is powered up with an external power supply.

1. Experimental Simulations

The prototype model and its simulation are divided into two parts. The first part deals with the authorized user and the second part deals with the unauthorized users.

Part 1: Authorized user:

In this case, the fingerprint is enrolled in the fingerprint module and when the user enrolls his/ her finger into it then the door of the vehicle opens and it shows "DOOR OPENS" in LCD shown in figure 6(a) and 6(b).

Part 2: Unauthorized User:

In this case, the fingerprint is not enrolled in the fingerprint module. So, if an unauthorized user tries continuously to open the vehicle door and puts his/ her finger into the module shown in figure 7(a) and 7(b). After 3 unsuccessful trials, the buzzer starts buzzing continuously and the GPS Tracker gets activated. It starts sending the location of the motion of the vehicle continuously and sends it to the registered Mobile number. (Owner's number). The Owner can find out the location by clicking on the link and choosing browse option which is shown in figure 8(a) and if he clicks on the link provided to the registered mobile number than it showed the exact location in the google map shown in figure 9. The browsing option will lead the owner into the Map and will navigate the whole motion of the vehicle. Figure 10 shows the complete hardware setup

CONCLUSIONS

The Biometric identification reinforces the vehicle security system by giving acces to selective authorised persons only. This system will enable only the authorised person to access the vehicle. In future the information can be directly sent to the police department along with a copy to the registerd owner. Tracking of the system through GPS has made the tracking system stronger. This security system along side the conventional Lock and Key is a reinforcement of security to avoid losing the vehicle.

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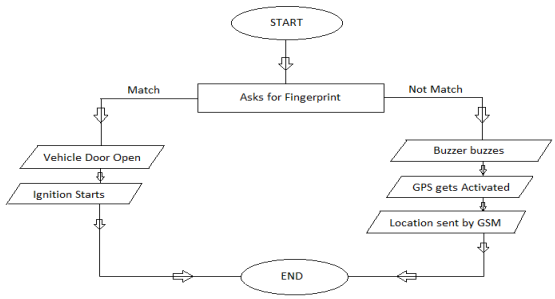

Fig 1:Flow Chart

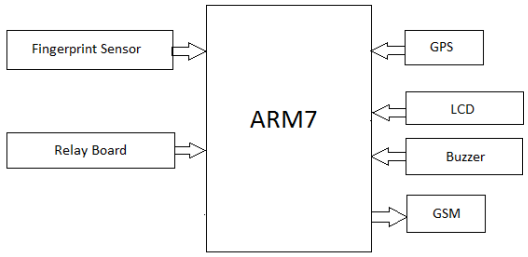

Fig 2: Block Diagram

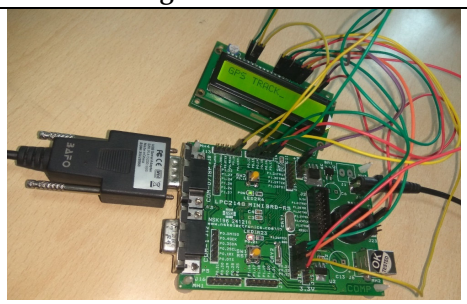

Fig 3: Interfacing of LCD with LPC2148

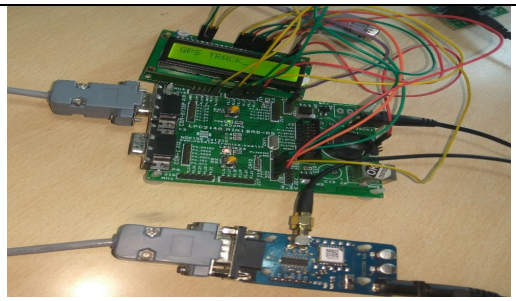

Fig 4: Interfacing of GPS with LPC2148

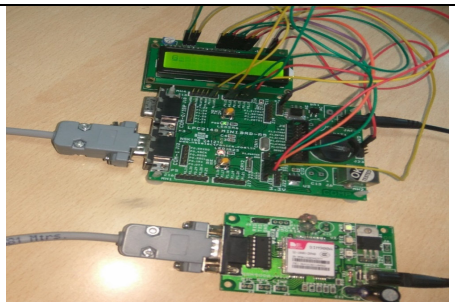

Fig 5: Interfacing of GSM with LPC2148

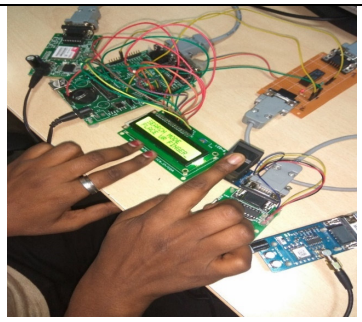

Fig 6 (a): Place Finger

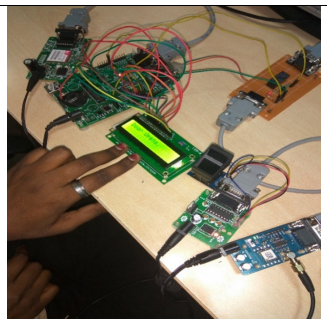

Fig 6 (b): Match Found & Door Opens

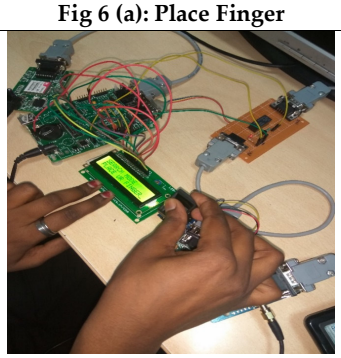

Fig 7(a): Place Finger

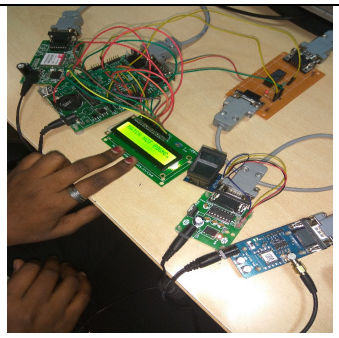

Fig 7(b): Match not found

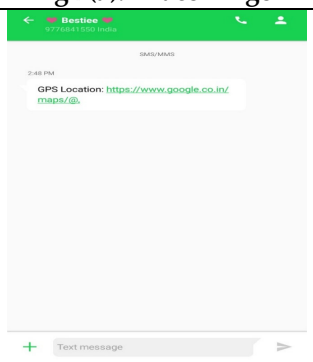

Fig 8 (a): Message Received

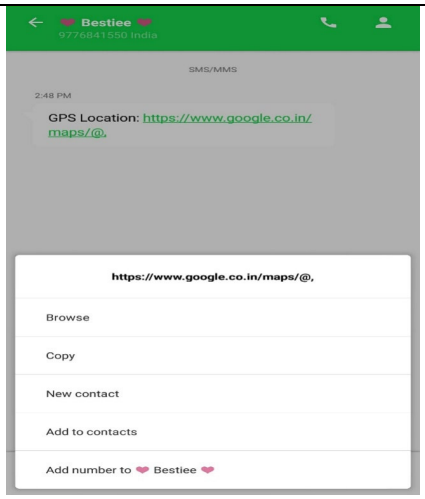

Fig 8 (b): Browse

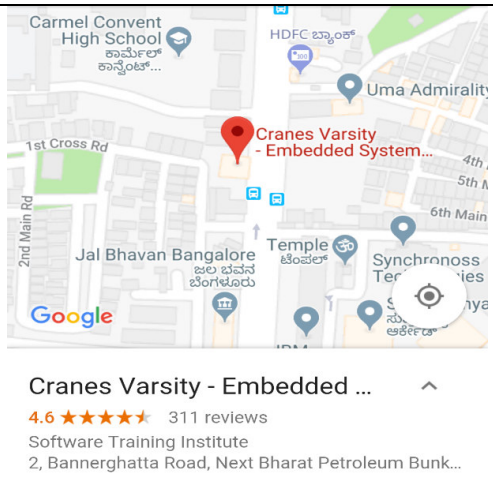

Fig 9: Map Diagram

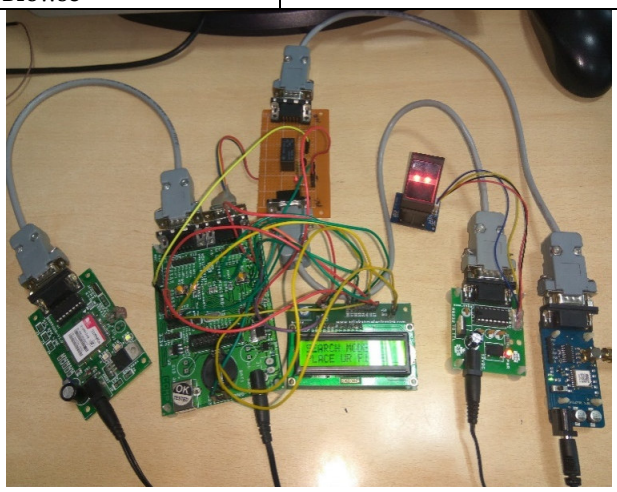

Fig 10: Hardware Setup

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RESEARCH ARTICLE

Smart Shopping Basket: An Application of Radio Frequency Identification Technique

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ABSTRACT

Marketing in malls and super market has its own advantages and dis-advantages. Advantages being able to choose as per will without constraints, getting the commodity immediately on payment etc. Dis-advantages being standing in a queue to make payments, have to carry the commodity in person etc. in this proposed model the billing process is simplified by completing the item scanning part of the task in the marketing basket itself. The payment can be done online through a reference number at the exit or may be done through portable swiping machine or even directly through mobile banking facility. This becomes more convinient for the customer and economic for the shopkeeper. Thus the goal of the article is very focused on reducing the waiting time during check out and ensuring customer comfort and satisfaction by cutting short the process of barcode scanning at the billing counter.

Keywords: market, economic, barcode, payment, customer.

INTRODUCTION

We see these days RFIDs are widespread and taking a role in many advanced projects due to its fast and effective response. RFID are general tags that are used for the unique identification of products by using radio waves. These RFIDs offer more advantages over conventional Barcodes as they have a major drawback which is Line of sight technology and also these barcode tags have constraints in its durability whereas the RFID tags are more durable and able to read/write data which could even be encrypted. These tags could hold plenty of data like product name, price, size, weight, and other information using their identification number. By implementing this RFID technology for a unique representation of each product in a market shopping is done more easily. This could be done by having a Shopping basket installed with an RFID reader to scan each product and load it which is controlled by a

microcontroller. When the customer is done shopping, they can pay by using ATM cards or by cash at the counters. Our concept satiates the expectation of customers whose basic demand is to ease the way of purchase. By regulating the RFID based shopping basket, one could easily bill the products themselves without bothering the presence of workers in the shop as details of products are readily available and displayed on the customer mobile phone. This outcome of the project will not only facilitate the customers but also the shop owners by eliminating the scanners and money spent on them.The controlling unit of this project is ARM7 LPC2129. The other components areinterfaced to the microcontroller. The components connected to the microcontroller areone RFID module, one GSM module. This project enables the customer to scan theproducts using RFID tags while placing them in the basket itself and when finishedshopping the customer can avail the bill in the mobile phone and pay the amount in thecounter directly. This project helps in reducing the queue in supermarkets and also savestime as scanning won't be done so the customer can directly pay and checkout.

LITERATURE REVIEW

Here we will cover the literature survey where various authors have done much work with the help of different technologies and a different controlling unit. Whenever shopping word comes in the individual mind, they spend more time as compared to the normal time in the shopping complex. This is because for buying any product we have to spend more time nearer to that area because of selecting a particular product. After selection process overs, then we have to move forward to the billing counter which again takes more time. Because no single person is standing in the queue, there are a lot many people standing in a queue which again takes more time. So to overcome these different technologies has been adapted in the shopping complex, such as RFID and Barcode.

Traditionally shopping complex uses barcode for the product and inventory tracking. RFID is replacing the barcode technologies because RFID is faster, with no requirement of the line of sight, it has both read and write capabilities, higher security [8]. As per the advantages RFID is used everywhere. Along with the RFID technology some others have used the Wi-Fi modules to send the billing information where a receipt is generated for the buyer using PIC microcontroller [9]. In [1] authors reveals that a system has been implemented to reduce the time required while shopping. This model is based on Raspberry Pi with Pi Cam which captures the video, Gear Motor & QR Scanner. According to the author [2], they implemented the system added RFID technology. In [3] smart shopping system is developed for blind people for whom purchasing the item will be quite difficult. So this system provides a way to the visionless person to but items in the shopping complex by using RFID technology [5].

The author in [4] focuses on a system in which the buyer puts any product into the trolley its details will displayed on the LCD. Based on the shopping list final billing reports get generated. Now here they have the option to delete some items from the list by removing the item from the trolley. These algorithms run on the Raspberry pi platform with the GSM module. A review ofthe smart Trolley system has been discussed in [7] in which the author has focused on RFID based shopping, smart trolley, automatic billing, smart trolley with automated billing.

PROPOSED METHODOLOGY

From the flowchart in Figure 1, it can be observed that the LCD connected to the main processing unit displays amessageis "Enter your number".By usingkeypadcustomercanenterthe10digit phone number manually. After entering the phonenumber LCDs"Scanyour items".Then scan the product one by one by showingit to the RFID sensor.Whiles canning the products,all theproduct details like product name,price, andTotal amount will be shown in theLCD. Ifaparticular productiss cannedeven several times then that particularproductis deletedfromthe billand the price of theproductisdeducted fromthetotalamount. And iftheproductisscanned an oddnumberoftimes then the productand price of that product are added in the bill. Once the shopping is completed the customer canpress thes

witch to end his/her shopping andtogeneratethebill. Afterpressing thes witchames sage willbe sent to the customer'sphone as well as to theadmin. The message containstheproductnameand theirrespective price,Total amoun talong with a unique bill ID.The message sentto admin contains thesamethingalongwith the customer's phonenumber to easyaccess.

The power source is connected to the micro controller to give sufficient powersupply for the smooth functioningof theproject.The16x2LCD is used to displaythe product name, price, and total amount, etc. The4x4 keypad is usedto enter thephonenumberof thecustomer.Theswitch is used to finish theshopping.The GSMmodule isused tosendthe message tothe customer whichcontainsthe product name, price, total amount, and unique Bill-ID.The same message is also sent to the admin alongwith thephonenumberof thecustomer.RFID is used to scan theproducts.

Simulation Results

Firstly, the whole system is power up and the LCD will display the Smart Basket on the LCD. After that through keypads manually enter the number shown in Figure 3(a) and Figure3 (b). Afterentering the number properly, LCD will display a message i.e."Scanyour items" shown in Figure 4(b). Then the customer needs to scan the item/productone by one by showingit to the RFID sensor shown in Figure 5(a). Whenever an item is scanned theLCD will displayits name alongwith itsprice as per the figure shown in 5(b). Afterdisplayingthe name and price, the LCD will displaythe total amount. Once the customer finishes his/her shopping he/she can press the button to end their shopping and generate the bill shown in figure .After pressing the button shown in figure 6.LCD will display a messagei.e. sending as shown in Figure 6(a).Oncethe messageis sent LCD will display a messagei.e. send shown in Figure 6(b). Both Customer and the admin will receive the same message on their phone which will havethename oftheitem/productalong with its price and at the end ofthe message total amount will be written shown in Figure 8(a).The admin can distinguish thebill of aparticular customer byusingthe billingid or the phonenumberof thecustomer, the phonenumberof the customer is onlysent to the admin message shown in Figure 8(b).

CONCLUSION

Theproposedmodelis user friendly. Time saving for the customers. Makes it flexible for all to use. Can be upgraded without any major hardware changes. No specific training required. Since RFID is used it will be quite low-priced. Since the system gets smart and autonomous the need of manpower can be reduced, thus benefiting the retailer by reduced man power. Since the envolvement of human is reduced the chances of human error and stealing of items the retailer also gains. This system would benefit the customers and the retailers at the same time as the number of customers served at the same time becomes higher.

Future Scope

This system can be further upgraded by the utilisation of more complicated algorithms and make shopping a better experience through automation. More updated controllers and programs can be utilised to improve the experience of customer and retailer.

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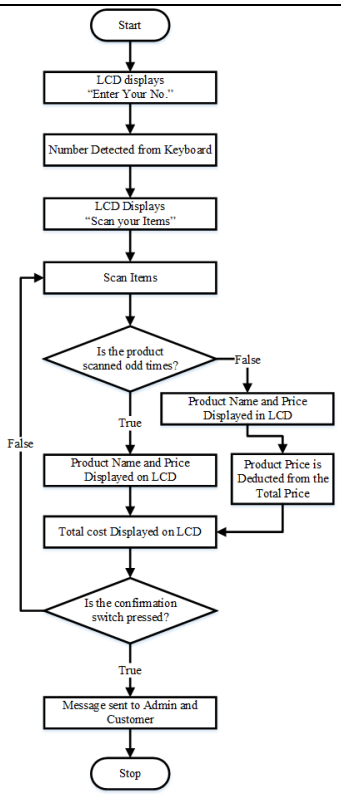


Fig1: Flow Chart

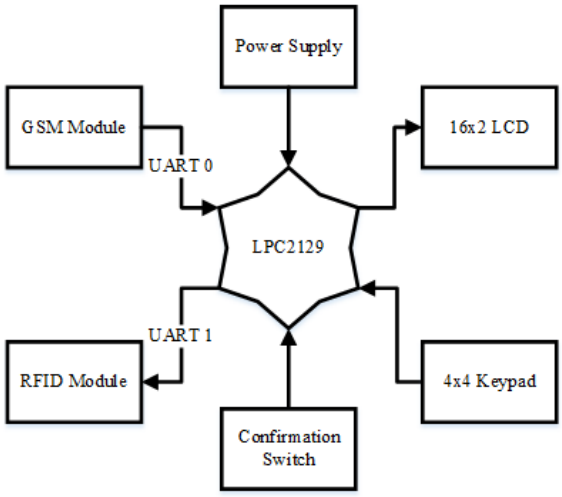


Fig 2: Block Diagram

(a)

(b)

Fig 3 (a)Display Smart Basket (b)Manually Enter Number

(a)

(b)

Fig 4 (a) Enter Mobile number (b) Scanning of Item

(a)

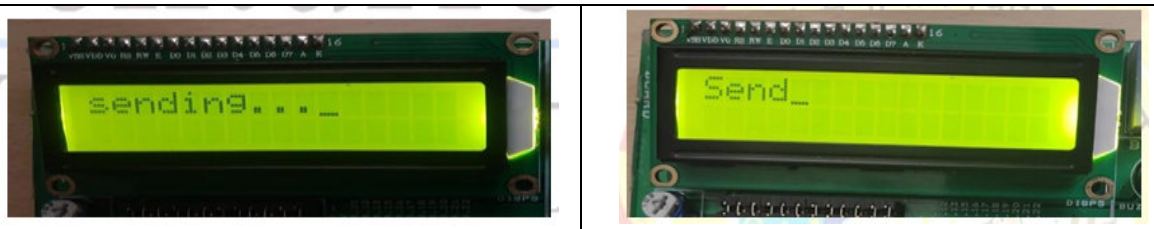
(b)

(c)

(d)

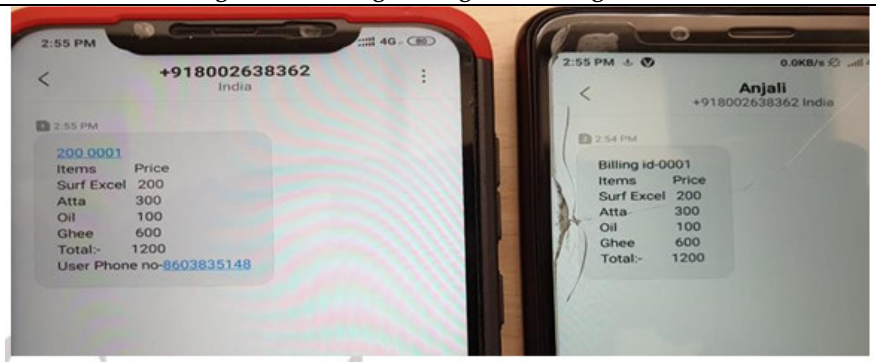
Fig 5 (a) Scanning the RFID Cards (b) Product Name & Price,(c) Display the Price of Individual Product(d) Display the Total Price of all the Product Purchased

Fig 6: Pressed Button after Purchase is over



(a) **(b)**

Fig 6: (a) Sending Message (b) Message Send



(a) **(b)**

Fig 7: (a) Billing Report Send to Admin Mobile Phone (b)Billing Report with ID Send to CustomerMobile Phone

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RESEARCH ARTICLE

Wireless Temperature Humidity Monitoring Controlling and Analysis of Multiple Room

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ABSTRACT

Appliance control has been quite painful ever since its existence. Wireless control is an unavoidable solution to it. IoT has provided us the technology to control them through a wireless medium. Along with the capability of remote control, if we can know the current status of the appliances along with the usage duration, it would allow users to effectively evaluate their consumption. Electricity is a valuable resource, wasting it without utilizing it properly. This article concentrates on the capability of technology to trace the usage, consumption, and remote control. NodeMCU along with Raspberry Pi working through the internet, using the open-source database server "PHP My Admin" installed on Raspberry Pi enables us to achieve the above-stated goals. This setup also operates over Mobile phones with the internet. The system uses the MQTT protocol to communicate with multiple NodeMCU and stores the relevant information in the server (in this case the Raspberry works as the database server and Node MCU works as a controller as well as a wireless data communication).The NodeMCU detects the temperature and humidity level through sensors and published them to the webpage as well as the SQL Server (Raspberry Pi) for entry into the database. This data is also displayed on the mobile device used for controlling thereby making the user aware of the current status and accordingly AC or Fan can be turned on or off. The system is employed with an optional AUTO mode to turn on the light and fans. This experimental set-up can be employed in educational institutions and offices to reduce the usages of electrical appliances which saves electricity.

Keywords: Electricity, database, device, temperature, remote

INTRODUCTION

The future is the age of connectivity, where all the appliances will be connected to the network. This technology will be takingover the control and monitoring work into its responsibility.The system is assigned with this responsibility to ensure comfortable and suitable working and living spaces for people. The wireless room automation is all about controlling and monitoring of indoor atmospheric conditions through controllers and sensors. All the communication of data and information takes place through a wireless medium like Bluetooth or Wi-Fi. Apart from this feature of temperature and humidity control other services can be implemented like entertainment, telecommunication, surveillance, etc. can be integrated into the system. Automation through IoT enables the user to access the appliance control through the internet via any mobile device having internet facility from anywhere in the world.In this article, an automation system is proposed to control the appliances remotely through a web-based interface using the internet. The main goal of this work is to implement a cost-effective interface to automate the appliances and monitor them remotely.

RELATED WORK

Monitoring and automation have been quite fascinating work in the field of IoT. Wireless sensor networks have been employed along with the IoT platform to perform much more complicated task like Air Quality Monitoring[1, 2], monitoring of industrial environmental conditions in Wineries and Creameries[3], some researchers have also employed this WSN technology to monitor the occupancy in an energy-efficient way by using PIR's and mathematical modeling to meet the needs[4].A similar type of work is proposed by designing a well-equipped room with a proper environment control system using WSN and Mobile agents [5].

PROPOSED METHODOLOGY

This system is designed to operate independently but the data is stored centrally. This information can be accessed for further analysis. The NodeMCU is the main operating brain for the individual control unit for the rooms implemented. The control system has been implemented in three rooms of our university viz Dean's Room, Room no 12, and Room no 10. The NodeMCU's are connected to the fans and lights. The main sensor is also connected to the NodeMCU which informs the control unit to take necessary action to maintain the standard comfort parameters inside the room. All the sensor information is sent to the Raspberry Pi which acts as a local server for storing the information in an open-source database i.e. MySQL shown in Fig 1.

The user of the respective rooms can observe the current condition and operate through a web-based application designed through HTTP and PHP. The user can use any device that has the capability of using the internet and a user interface with a web browser. The individual controller has its web-based application. The Raspberry Pi is also equipped with a similar type of app that can monitor all the controllers at the same time. The NodeMCU is the control unit to be installed individually in every room under consideration. Here in this experimental set-up, three rooms are taken into consideration, the Dean's Room, Room No 10, and Room no 12. Each room is equipped with a DHT11 module to monitor the Temperature and Humidity as shown in figure 1.

Each NodeMCU is programmed and associated with its dedicated Web-Based Applications to monitor and operate independently. It is programmed to take the sensor readings and update them into the database. Then compare the data from the database with the desired parameters and operate the appliances (Fan and Light) the lights are user-controlled as its an official set-up but the fans can be controlled by the controller directly. The controller actuates the appliances through a relay module connected to it as shown in figure 2. the relay module used in this project ate Active Low triggered, hence the NodeMCU has to give a low signal to activate an appliance.

The complete connection of the project is as described graphically in figure 3. Here it can be observed that the fans and lights are connected through the relay module, the sensor is connected to the NodeMCU. The controller is connected to the internet through the router. The Raspberry Pi operating as the local server equipped with the open-source SQL server "MySQL" is also connected to the internet through the router. And all the information is stored in the database server through the internet. This stored data can be accessed by the user through the internet using any handheld mobile devices or desktop provided they have internet access and have a GUI to operate the Wen Based Application.The commands are passed on to the controller through a user interface designed through HTTP and PHP. The interface is password protected as shown in figure 4.

The page is secured to avoid any unauthorized access. Upon successful login, the interface directs the user to open the page corresponding to the room to access as shown in figure 5. The data from the controllers are transferred into the local SQL server as shown in Figures 7, 8, and 9. The respective information from the controllers in the rooms is saved here in a very organized manner for further access and analysis. This information contains the data from the sensor and the status of the appliances, i.e. for how long they have been in operational condition with a corresponding timestamp. The data is posted on an hourly basis taking into consideration the standard duration of a classroom lecture. The Raspberry Pi operates like a local server to the experiment and stores the information and provides them as needed to the NodeMCU and the user.

RESULT AND DISCUSSION

Upon analyzing the database and plotting the curve from the available data for an individual room the following plots are obtained as shown in figure 13, figure 14, and figure 15. Analyzing the plot for the Dean's room it observed that the temperature and humidity are staying quite stable and constant as the number of visitors to Room 1is quite limited.Similarly analyzing the plot for room no 10 it is quite clearly observed that thought temperature level remains quite stable due to the usage of Air Conditioner the humidity level has quite a few spikes when the number of occupants changes inside the room.Observing room no 10 it's observed that the increase in student strength increases humidity level inside the room due to the hot climate. But the Air Conditioner quite significantly struggles to bring the temperature down resulting in reduced humidity but fails to bring the temperature down.

CONCLUSION

From the experimental set-up, it became quite clear that this system of room monitoring, controlling through IoT is quite user friendly and informative in accumulating data related to the environmental parameter inside a room.Using this method, it can be made possible to track the usage and wastage if electricity at the workplace.This system can be further upgraded to operate the Air Conditioner and lights in a fully automatic mode. It can be scheduled for classrooms and operate automatically without the intervention of the user. This would enable the practice of controlling the wastage of electricity.

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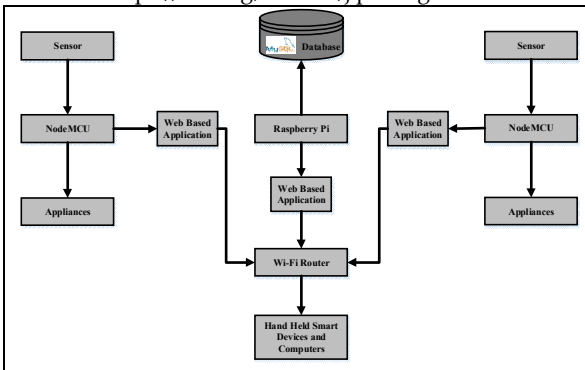

Fig 1. Block Diagram

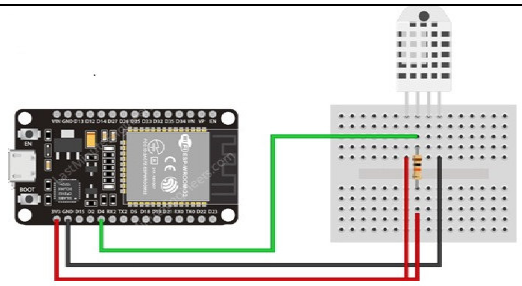

Fig 2: Interfacing of DHT11 with NodeMCU

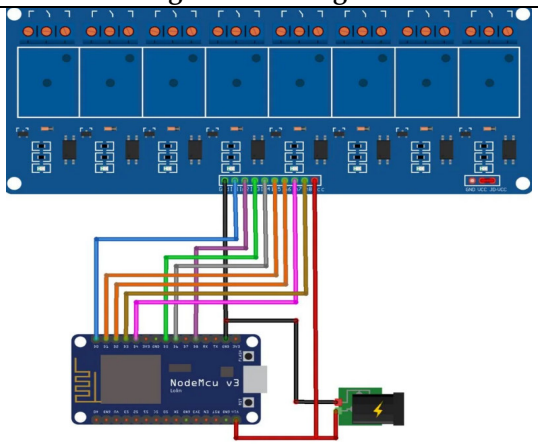

Fig 3: Interfacing of Relay Module to the NodeMCU.

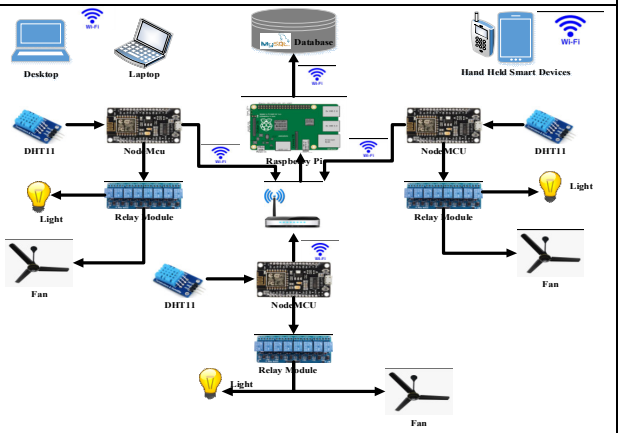

Fig 4: Graphical Representation of Complete Project

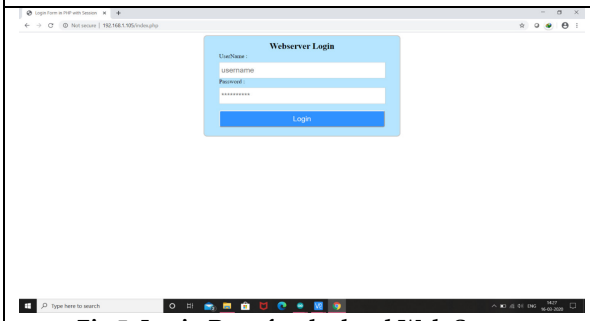

Fig 5: Login Page for the local Web Server.

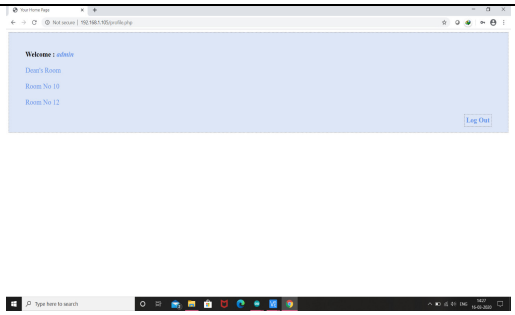

Fig 6: Dashboard to select the room under consideration

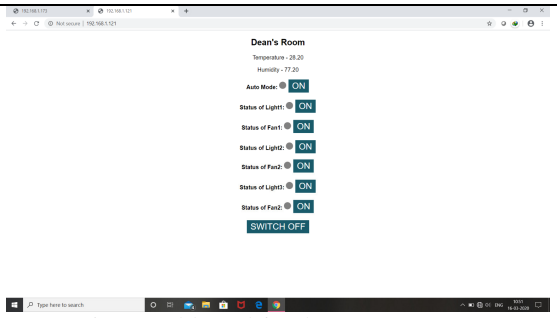

Fig 7:Dashboard for the Dean's Room

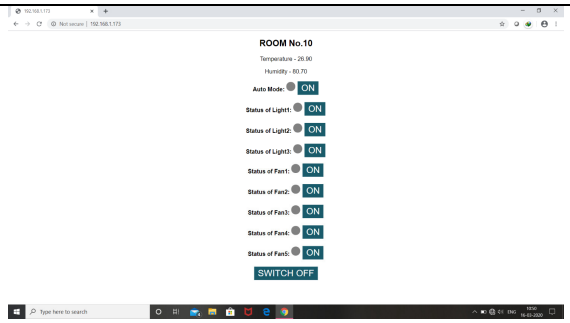

Fig 8:Dashboard for Room no 10

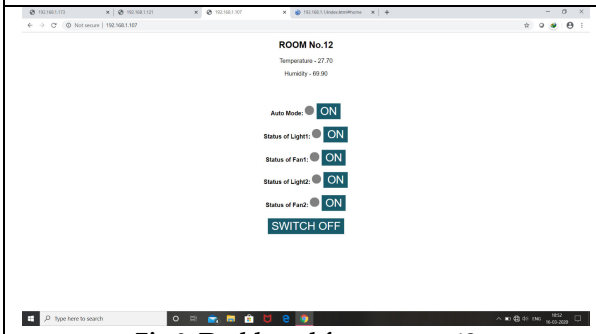

Fig 9: Dashboard for room no 12

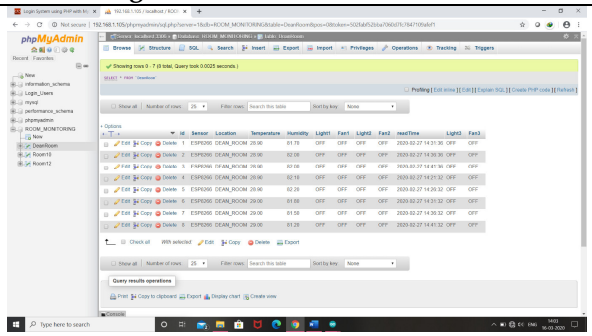

Fig 10: Controller information for Room 1

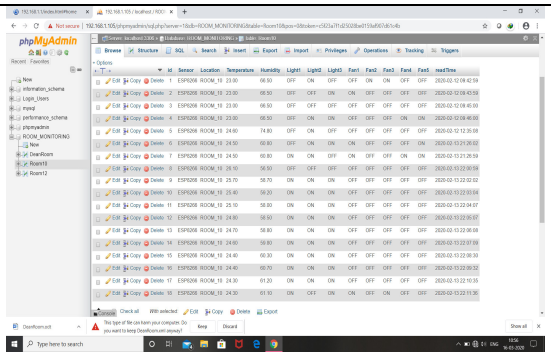

Fig 11: Controller Information for Room 2

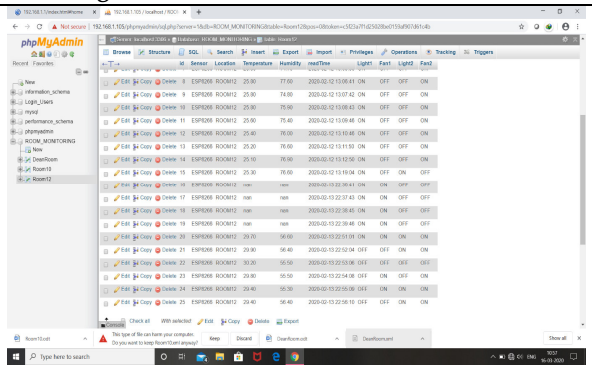

Fig 12: Controller Information for Room 3

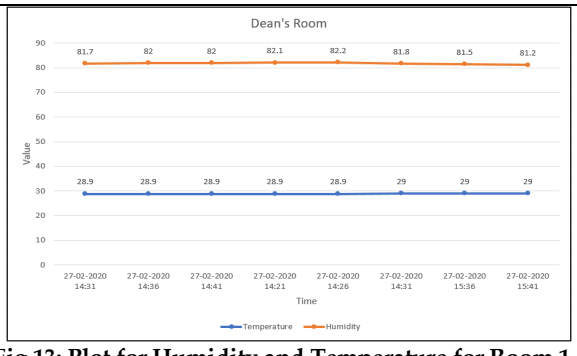

Fig 13: Plot for Humidity and Temperature for Room 1

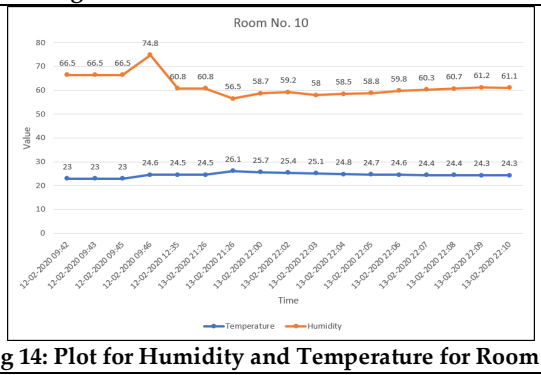

Fig 14: Plot for Humidity and Temperature for Room 2.

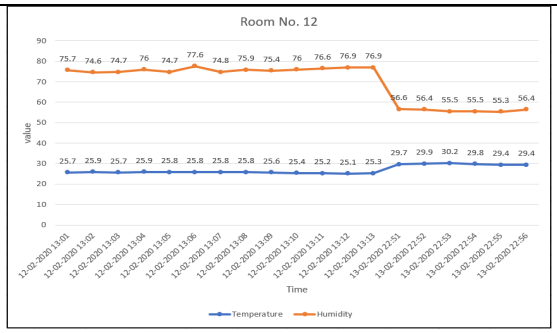

Fig 15: Plot for Humidity and Temperature for Room 3

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RESEARCH ARTICLE

Voiced Based Electronics Guidance System for Visually Impaired Pedestrians

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ABSTRACT

This articleis targeted to investigate the aid forthe mobility of blind and visually impaired people. It is supported by a processing unit called LPC2129 with synthetic speech output. This system is also comparatively low cost, small, portable, and provides information about the routes to the user which aids in making decisions. The system is provided with sensors like ultrasonic and vibrator to reduce the outdoor walking difficulties of the blind man. The proposed arrangement detects the nearby obstacle via stereoscopic sonar system and a vibrotactile response is sent back to inform the visionless people about its location & warn from the nearby vehicle. The foremost observation of this paper is to produce electronic support as guidance to overwhelm the lacking of visualization power by proposing an easy, safe, cost-efficient, customizable guidance system for the visually impaired. The suggested electronic system senses the obstacles in its path by transmitting the ultrasonic waves through the ultrasonic sensor. This CPUreceives the signal from thesensors,performs few calculations,and then it alerts the blind pedestrians through a sound and also with a vibration. One of the advantages of the proposed system isits voice-based announcement for straightforward navigation which can assist a blind pedestrian to undergo a busy road. Moreover, this system is an acoustic guidance system for the visually impaired pedestrians using the transformation of ultrasonic-to-audio signal.

Keywords: LPC2129, Ultra-Sonic Sensor, Vibrator motor, Visually Impaired

INTRODUCTION

Blindness is the loss of temporary or permanent sight. This condition of someone creates difficulty with normal daily activities like driving, reading, socializing, and walking. And also reduced vision isn't corrected by glasses or contact lenses. Globally the reason for visually impaired is refractive errors, cataracts, and glaucoma. Even there are plenty

of disorders that will cause sight problems are age-related devolution, diabetic retinopathy, corneal clouding, childhood blindness, and number of infections.

Screening is the techniques for vison problem which can help individuals to enhance their future vision. 80% of the visually impaired person which is estimated by the globe Health Organization can either be preventable or curable with treatment, but people are avoiding visiting the attention test. From the literature, within the year 2015, 940 million people with vision loss, 246 million with low vision, and 39 million were blind[1]. But since the 1990s the visual disorder rates are decreased.

There are classifications of visual impairment based on the World Health organization are given below in Table 1.There are different strategies available to address vision impairment which is very much cost-effective and feasible to implement. Over the last few years, WHO has established and executed several tools to upkeep countries to estimate the provision of eye care services. They are 1) eye care services assessment tool, 2) Tool for assessment of diabetes and diabetic retinopathy, and 3) Tool for assessment of rehabilitation services and systems. World Health Organization has also developed the World report, these reports focused on ensuring comprehensive and integrated eye care in countries. From the technology perspective [2], people with vision loss use two broad categories 1) General Technology and 2) Assistive Technology. General technology covers computers, hand held devices, GPS, and GSM devices. But assistive technology is aimed to aid people with vision loss or other disabilities including screen readers, video magnifiers, and other devices for reading and writing. Though there are different steps taken by the government for the visionless people. This paper will talk about how technology can help the blind pedestrian to cross the road or walk through anywhere at any time. [3] According to the World Health Organization, 270,000 pedestrians face severe accidents on road every year. Moving safely is the fundamental right for everyone. The feeling of insecurity among everyone mind mainly the old and the blind people causes them to stay at home which reduces mobility.

The risk for the pedestrians is both from driver's behavior and infrastructure.Behavior is related to the speed of the vehicle, mobile phone use during driving, alcohol, and drugs. Infrastructure may be related to roadway design and lack of visibility. To make visual impaired people travel independently mainly uses auditory and tactual information. When an obstacle is detected in the close vicinity of the the sensor it sends an information to the vision impired person in the form of sound and vibration.The main concept of the paper is to provide an electronic aid as guidance to overcome the lacking of visualization power by proposing a simple, efficient, electronic guidance system for blind and visually impaired pedestrians. It is a helping aid to blind people for their navigation through a busy environment. The system will sense the obstacles for the person and will give alerts with sound and vibration. The blind person can carry a stick to get rid of the accident-prone Zone.The different system has been developed by different people to help blind people. The paper is organized as follows; Section 2 presents the literature review on implementation of various techniquesfor vision-impaired people, Section 3,discuss the proposed methodology,Session 4 highlights hardware and Software used implemented to implement the system, in Section 5 presents the simulation results, Session 6 Concludes with discussing the future work and suggested techniques which may be advantageous on application.

LITERATURE REVIEW

This section deals with various types and levels of work done for the safety of blind people. As [6] we know that there are more no. of blind people in the society, who suffers from traveling. The various technological blind stick has been developed for the safety of the blind people so that they can walk easily on the road. The authors focus on electronic technology which uses PIC microcontroller, 3 ultrasonic sensors, and buzzer, to provide fully automatic obstacle avoidance with notification in the form of voice [1]. Here the simulation and PCB design for the system is done through Proteus v7.8. This is a very vital step that an author has taken to design and implement the circuits

before it comes to real hardware use.In the next paper author [2] proposed a simple, cheap, user-friendly, smart system that improves the mobility of visionless people in the specific area. They have used PIC microcontroller, infrared sensors that emit IR waves and scan a predetermined area surrounded by blind people. This system calculates the direction and distance of the objects and alerts the user about the obstacles shape, materials, and direction.

As we know that the technology is moving and changing very fast, based on the technology advancement here author [3] describes the smart stick for the blind person. This stick uses technologies like PIC 16F877, GSM, LDR, Android application, ultrasonic sensor, Facebook server, and Bluetooth. The switch with an emergency functionality can help the user to communicate with their relatives through voice calls or SMS. They reveal that onboard implementation will be more efficient and accurate and more convenient to use.

Now the paper [4] proposed an Arduino Nano, Bluetooth, ultrasonic based obstacle finding stick for visionless people which helps to detect the path using an ultrasonic sensor and MIT Android App. And also informs the blind person about the circumstances and present condition of the path. Many papers developed the smart and blind stick based on sensors and Arduino variants for visually impaired people. The system was designed, programmed using C Language, and tested for accuracy and checked, which can detect obstacles within 2 m [5]. The study in [7] proposed the sensor-based stick for blind people. Here the main objective is to develop a system which can detect the object in various direction, detecting pits, and manholes on the ground to make free to walk for the blind people. This system uses multiple sensors with features that are used to detect the obstacles. The prototype system modeling is done in Pro/E creo 5.0 Software.

The external battery used can be recharged through solar panels for instance.The main objective of the paper cover in [8] is to provide a voice-based intelligent system that assists blind people by using an ultrasonic sensor and Infra-Red sensor. The prototype stick is capable of detecting obstacles in the range of 4 meters and gives a suitable message to blind people to move twice the normal speed. Here the author has used the PIC microcontroller which uses the ADC to convert the Analog value received from the sensors connected to the system. The whole programming uses the embedded C programming language. They have also taken the help of the Proteus simulator tool to do the simulation of the whole circuit. The main objective of this paper is to focus on LPC2129 based ARM7 Processor, GSM, GPS, Ultrasonic Sensor, Switch, and buzzer and vibration sensor to help the blind people to move freely. He a device can be designed for blind people that help them to travel independently and also it must be comfortable to use.

PROPOSED METHODOLOGY

The proposed system is designed to collectinformation about the environment via ultrasonic sensors and extracts the information. Thisinformation obtained is then transformed into an audio signal after justified calculations and processing due to which the blind pedestrian can interprete the surroundingsthroughthe sound generated by the system. The entire operation of the project is described by using a diagram which graphically explains the method and concept as shown in figure 1. In this figure all the components used to perform the experiment is shown.
The figure 2(a) figure 2(b) shows the communication between the various modules used in the project and how the various modules communicate and the operation flow respectively.

In the proposed model the circuit is assembled and the program is executed. The Panic button and Ultrasonic sensor are acting as interrupts connected to the Centeral Processing Unit for immediate sensing and responding to the environment. Here the ultrasonic sensor is producing the waves continuously. When the obstacles come into the vicinity of the sensor then it creates a vibration and buzzing sound. In case of panic, the switch is pressed interrupt 1 gets activated and data from the GPS receiver is collected and then the data is sent to the blind person's family

member through the GSM module. The LCD is used to display the longitude and latitude received from the GPS receiver before sending them to the family members. In case of ultrasonic sensor receives the presence of an obstacle then interrupt 2 is activated and the blind person is alerted with the help of a buzzer and a vibrator about the presence of the obstacle. In the case of encountering an obstacle, the LCD will show the presence of the obstacle.
The alerting system consists of dc motors that can be moved at different speeds for providing the sensation about the obstacle. In the case of any emergency, the blind people can alert his dear one by simply pressing on a switch. The GPS module connected in the system will locate the blind man's position and a message is sent using a GSM module.

Use of Hardware & Software

In this to develop the system-specific microprocessor cores and a family of tools, libraries, and off-the-shelf components are used. ARM is one of the important options available for Embedded System development. It is developed by ARM Holdings and based on RISC architecture. It works on 3.3 v as compared with the Arduino variants. The use of the ARM processor reduces costs, heat, and power use. LPC2129 Microcontroller is one of` the widely used Integrated Circuits from the ARM-7 family. It has 40 KM of RAM, 512 KB of ROM, 10 bit ADC, DAC, timers/Counter, ISP, VIC support and CPU operating voltage range of 3.0 V to 3.6 V. There are multiple pins used for a different purpose related for the prototype model development Table 2.

GSM

GSM is the most commonly used mobile communication system. It operates at 850MHz, 900MHz, 1800MHz and 1900MHz frequency bands. It uses TDMA technique for commumication. It digitizes and sends the information in 2 streams of data in a specific time interval. It has a capacity of 120Mbps information handling rates. Its associated with a sim card, upon receiving the digit command it sends the information through SMS.

GPS

A Global Positioning System, otherwise known as GPS is designed to assist navigation on land water and air. There are GPS satellites in the space to triangulate the location and send the coordinates to the GPS sensor. That information is received by the controller and processed in to an interpretable format for the user. A network of 31 satellites covers the entire earth surface. The coordinartes are triangulated by calculating the distance form atleast 4 satellits and the coordinates are calculated.

Ultrasonic Sensor

An ultrasonic sensor is a device that works on the principle high frequency sound travelling through air and receiving of reflected sound waves getting received by the sensor. By calculating the time difference the distance of the reflecting surface from the origin can be obtained.
The expression for the above explation is as below:
Distance = (high level time * speed of sound (340M/S) / 2).

DB9 Connector with Cable

It is an analog 9-pin. It is mainly used for serial connections, allowing for the asynchronous transmission of data with a standard RS-232 (RS-232C).These are used to change the cable connection type shown in Fig 3. They can easily be soldered to a custom length cable creating a durable connection for all applications. These connectors are made with high-quality materials to ensure durability and long life. The kit includes the crimp connector, crimp pins, a plastic hood, and all hardware.Here DB9 Connector was used for two purposes, 1) for dumping the code into LPC2129 and 2) for Connecting GPS and GSM to LPC2129.

EXPERIMENTAL RESULT

The main aim was to help the blind people when they come out alone on the road. A test model or we can say a tabletop model has been developed. The process is as follows in two steps.When the panic button is pressed the code is dumped into the controller using USB to UART converter cable.After the reset button is pressed the program starts running displaying BLIND NAVIGATION the name of the project in Fig 4 and waits for the inputs which are connected as interrupts to pin p0.03(Switch) and p0.07(Ultrasonic Sensor). The16X2 display is used in an 8-bit mode to show the simulated outputs on it.In the real project, the LED will be replaced with a buzzer for the warning, and the vibrator will be connected for vibration feedback.The GSM and GPS modules are connected using DB9 connecter cables to the UART0 and UART1 of LPC2129.]

Then it enters an infinite WHILE loop where it waits for the input from the user, the input here is the switch which acts as the PANIC BUTTON shown in Fig 5.After the PANIC BUTTON is pressed the GPS function is called which collects data (longitude and latitude) from the GPS receiver and stores them in the assigned arrays shown in Fig 6, Fig 7 & Fig 8. The Lattitude data received is 1255.5618,N,is stored in array latt[ ] and the Longitudinal data received is 07736.0066,E, is stored in array long[ ]. The data from the GPS model is sent to the family members through the GSM module to the mobile phone shown in Fig 9.

The second part is when an obstacle is detected after the reset button is pressed the program starts running displaying BLIND NAVIGATION the name of the project. Then it enters an infinite WHILE loop where it waits for the input from the user, the input here is a high pulse from the ultrasonic sensor when an obstacle is sensed shown in Fig 10& Fig 11. When an obstacle is sensed, it enables a buzzer and vibrator. A vibrator is used to give feedback to the blind person in the form of vibration and buzzer is used to alert person by giving a buzzing sound.After alerting the blind person about the obstacle with the help of a buzzing sound and vibration feedback the code returns into the infinite while loop and again waits for the interrupt to happen. And when there is no obstacle then again it will come to the infinite loop.

CONCLUSION

This navigation system for the visually impired converts the environmental information of the up-coming obstacle into electrical signals. These electrical signals are then converted into equivalent audio signals and ill-vision person gets an information of its surrounding. Based on the audio signals the pedestrian can navigate with ease through the roads. If in-case the pedestrian with vision issue feels an uncomfortable situation he or she can push the panic button that will immediately take the GPS location from the sensor and write an SMS having the coordinates. Here the GSM module plays its role to process the SMS and send it to the near and dear ones. This will inform them of the location of the user so that the person can be tracked through the coordinates supplied. More sophisticated sensors and with higher range can be used to help them have more information hence a safer navigation through the roadways. The experimental set-up can be further upgraded to utilize a camera and convert the surrounding images into electrical signals and feed them to the nervous system giving the vision less person a virtual vision.

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11. https://www.inclusivecitymaker.com/pedestrian-safety-visually-impaired-blind-people/

Table 1: Classification of Visual Impairment

Sl. No.	Eye with Best Possible Glasses Correction	Description
1	20/30 to 20/60	Mild vision loss
2	20/70 to 20/160	Moderate visual impairment
3	20/200 to 20/400	Severe visual impairment
4	20/500 to 20/1,000	Profound visual impairment
5	More than 20/1,000	Near-total visual impairment
6	No light perception (NLP)	Total Blindness

Table 2: Pin configuration for connected Devices

Sl. No.	Pin No.	Connected Devices with description
1	**P0.03**	**Interrupt pin for the panic button.**
2	**P0.07**	**Interrupt pin for an ultrasonic sensor**
3	**P0.15-P0.22**	**Display data pins D0-D7 of LCD**
4	**P0.10**	**Display enable pin of LCD**
5	**P0.13**	**Display register select pin of LCD**
6	**P0.25**	**Connecting Buzzer**
7	**P1.16-P1.17**	**Input for the motor driver (Vibrator).**
8	**UART0**	**GPS receiver connection.**
9	**UART1**	**GSM module connection**

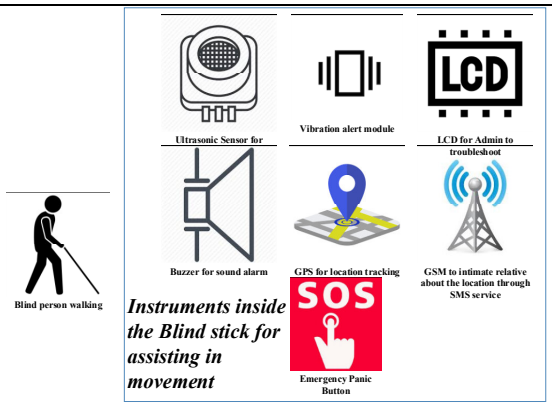

Fig 1: Prototype Model General Idea

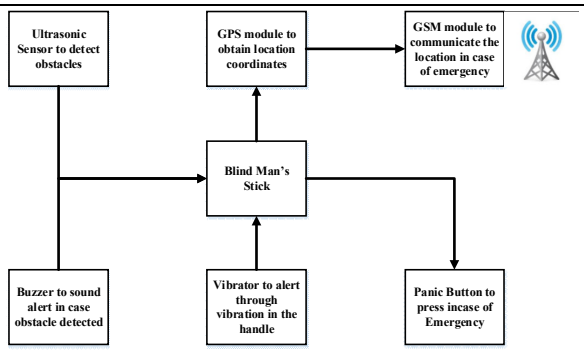

Fig 2(a): Block Diagram

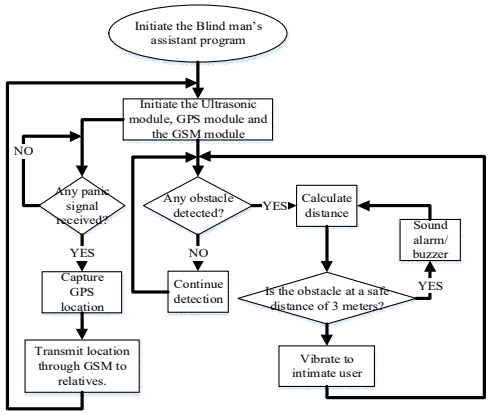

Fig-2(b): Flow chart of the operation.

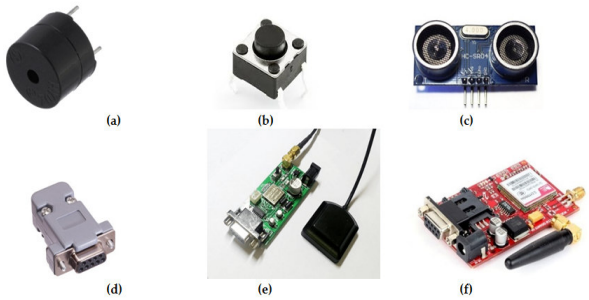

Fig 3: (a)Buzzer (b) Push Button (c) Ultrasonic Sensor (d)DB9 Connector, (e) GPS Receiver, (f) GSM Module(SIM900A)

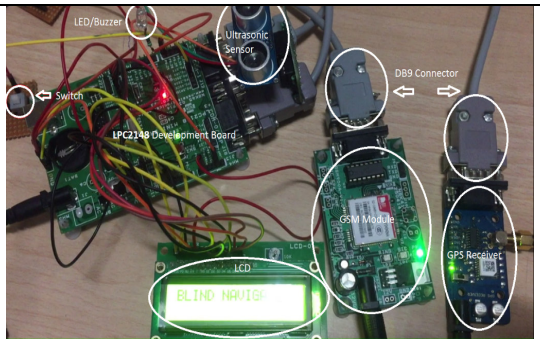

Fig 4. Final setup during Initialization

Fig 5. Waiting for the User Input

Fig 6: Panic Button is Pressed

Fig 7: Latitude Message on LCD

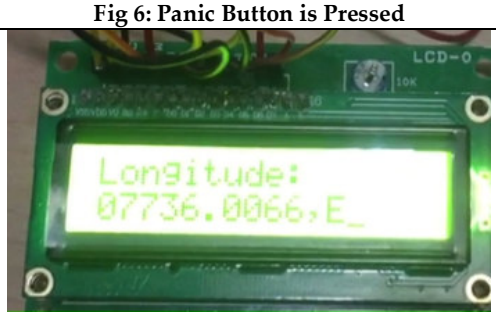

Fig 8: Longitute Message on LCD

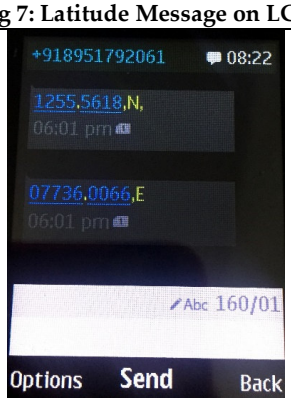

Fig 9: Message on Mobile Phone

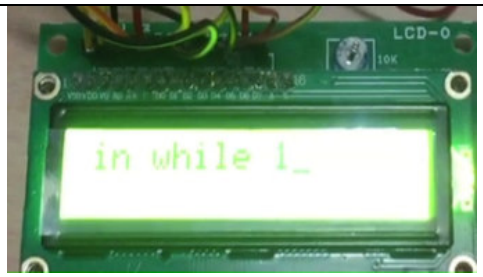

Fig 10: Waits for Ultrasonic Sensor to Trigger

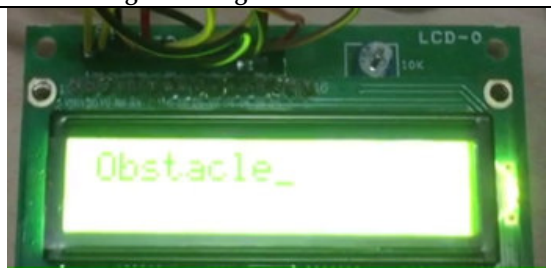

Fig 11: Obstracle detected

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RESEARCH ARTICLE

Self-Driven Metro and Biometric Reservation System using ARM Microcontroller

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ABSTRACT

This article is designed to demonstrate the metro technology used as a prime mode of transportation in the developed countries. These trains are equipped with an auto-pilot option that enables automatic running of the train from one station to another. Though it is known as auto pilot, actually human intervenetion is required to enable and disable this feature.The proposed system is supposed to eliminate the need of human intervenetion. The system uses an LPC2148 microprocessor thar belongs to the family of ARM 7. The metro platform equipped with the small tools i.e. the IR sensor modules. The IR sensor installed in the platform triggers the train stop sub-routine. Then the sub-routine for opening the door of metro is executed. The passangers can now board the train. The door sub-routines closes the door after a specified time period. The compartments are also mounted with sensors that counts the number of passangers boarding and de-boarding the trains. The train closes the door when the maximum occupancy level is reached even if the allotted time for the door is not over. An alert is triggered just before the door closes. The train repeats the process at every station. This system is further enhanced by making the control system display the status for the passangers convenience. This status display consists of arrival and departure timings for each upcoming station.

Keywords: LPC2148, IR Sensor, DC Motor, LCD, Buzzer

INTRODUCTION

Train travel is one of the economical mode of public transportation. Train being slow the Metro train is the alternative to train travel as a faster mode of transportation. Its faster, safer and economical mode of public transportation, in the modern days. The driverless metro train allows a significantly secure and high-performance

means of transportation. The proposed system makes use of a microprocessor to control the movements of the train. This system has the feature of counting the number of passangers boarding and de-boarding the train. The counting system controls the opening and closing of doors. The proposed system also comprises a collision avoidance systemincase two trains are directed on the same track. The distance between the stations are pre-defined so they can operated without human intervention. The system is enabled with an emergency switch for emergency braking of the train.

Rail transportation means transferring huge no. of gods and humans from one place to another. Booking of railways tickets is becoming more concern because of the increased rate of the population. Earlier individuals used to stand in a queue to get tickets. This method was very much time taking. To overcome this various mechanism has come across to provide comfort to the individuals during ticket reservation. One important method is to use the biometric-based ticketing system [1], RFID based ticket reservation system, and fingerprint-based ticket reservation system. All the mentioned technologies use a unique identifier for each individual. The whole process consists of starting from registration to booking and validating on the date of the journey. But RFID [4] system type of reservation system is much more complex and has a drawback. This is because an individual has to carry the RFID tag during the time of Journey and it creates problems if in-case by any means the individuals forgot to carry the tag [7].Many have used GSM, GPS, ZigBee, and RF technology [8].

The study of each technology brings an improved solution to the society in terms of cost, convenience, user satisfaction, and future implementation. Based on the technology one has to select which suits the common public and visionless people. Some literature generates a ticket printing system with the help of QR code [2] for the passenger. While implementing the prototyping model they have to make use of different processors and controllers and different peripheral devices like Raspberry Pi, ATmega 16, printers. Arduino etc. Going towards the deeper literature survey, we found that few papers use face recognition [6] system for fare calculation deduction system utilizing the automatic system using a camera. The above technology helps the individuals save time required for ticket reservation and also increase the accuracy level of the tickets which is performed daily. The different country like the UK has adopted smart and integrated ticketing Technology. In that paper, authors have suggested both the legal and commercial risks associated with the ticketing system.

PROPOSED METHODOLOGY

The proposed methodology consists of two parts the first part tell about the Flow chart and the 2nd part tells about the block diagram of the proposed system. The Flow chart gives overall idea about the weather system that is developed using LPC2148 and GSM module. In simple words it can be explained as when the GSM module is turned on and the network is available it waits for the message and when the message is received it matches with the code word if it matches exactly when it will since the surrounding area's temperature and humidity and sends the data to the sender of the message. If the signal is not available, it waits still it gets signal. If the received message is not matched, it will send a response saying "try again" to the sender number. After completing one cycle it again waits for the next message to come. This process is repeated continuously.
The fig 3 represents the communications between the different components of the project. The micro-controller is LPC2148 it communicates among IR sensor, LCD, and DC motor. IR sensor communicates between motor and LPC2148 Board. The IR sensor will send the interrupt signal to the LPC2148.

Hardware & Software Description

This work consists of the following hardware LPC 2148 Mini Board, LCD, DC Motor Driver IC, DC Motor, IR Sensor, Jumper Wire, Buzzer, Power Supply (12v adaptor), and Fingerprint Sensor.
Microcontroller Board:LPC2148 mini development board is used to develop the prototyping model.

Motor & Motor Driver Circuit: Dc motor is used to drive the metro train.
Sensor Module: Basically will concentrate on the IR sensor, Fingerprint Sensor, Buzzer as an input, and output devices connected to the main processor unit.

Fingerprint Application
The above figure is called as Fingerprint Application. Here, we can enroll new fingerprints and also can delete the older ones. To make this application run, we need to follow the steps:

- Open Device (O)
- Choose the COM Port (identifying it from the Device Manager)
- Enroll (add new fingerprint)

This above step will help to add a new fingerprint.
Further, we can use Search option to find whether the fingerprint exist or not.

Flash Magic: This is a utility application which is used to upload the hex file into the microcontroller board through the UART port. From the figure we can see that it consists of 1) option to select the microcontroller, 2) COM port, 3) Baud Rate, 4) Interface 5) Oscillator Frequency, 6) Browse for hex file. 7) Start to upload the hex file. This is done by serial communication using UART (Universal Asynchronous ReceiverTransmitter) by connecting PC with UART0 of microcontroller using RS232 (DB 9 cable) connector.

Simulation Results

The below algorithm gives an idea of how the setup works for a single run of the code.
Step1: Firstly include all Header files.
Step2:Declare different functions used and global variables.
Step3: Include delay functions file and LCD related files that are being used.
Step4: The main function is started and different variables used in the program are declared.
Step5: Motor pins were declared.
Step6: Interrupt pins were defined.
Step7: Wheel motor pins are made high for the running of the metro wheel.
Step8: When an interrupt is occurring for the 1st IR then the wheel motor pins are made low and the door motor pin is made high.
Step9: Then 2nd and 3rd IR sensors are continuously monitored and person count is maintained.
Step10: After 30 seconds or if the person count reaches maximum whichever is earlier, the buzzer will beep, and simultaneously the door motor pin will be made high for opposite direction movement.
Step11: Then the wheel motors are made high again.
Step 12: It will continuously check for step 8 and if an interrupt occurs then it follows the same flow again.
The fig 7 represents the interface between the Finger Print Sensor (R305)Module with LPC2148 Microcontroller. Here we have connected the RX and TX pin of using UART pins of LPC2148.It is scanning the fingerprint and matching it with the database saved earlier.

Figure 8 shows that the fingerprint given, matches with a record present in the passenger database. The figure 9 and 10 shows that after a match is found in the passenger database it displays the passenger information and successful booking of ticket message is printed up respectively. The figure 11 shows the LCD shows the required fare for travelling to the destination and that much amount is deducted from the passenger account. The above figure 12 shows that if any unauthorized person is trying to book a ticket and record is not found in the passenger database then it denies and show that no match was found. The above figure 13shows that in normal condition the metro wheels are rotating and the door motor is in the stop position.
The above figure 14 shows that after the interrupt is raised for the 1st IR sensor then the wheel motors stop rotating and the door motor starts rotating for 2 seconds. The above figure 15 shows that after the door is open it will continuously monitor the 2nd and 3rd IR for monitoring the person count i.e. incrimination and decrimentation of

person count. The above figure 16 shows that the door will be open for 30 seconds and simultaneously wait for the maximum number of person count and whichever occurs first, then the buzzer will beep and the door will be closed and the door motors will start running again.

CONCLUSION

Its clearly evident from the experimental setup and the operation that it works quite well in the model. Use of the IR sensors can be replaced by by industrial sensors as we know that though IR sensors are rugged they are sensitive to sunlight and might work eratically. It runs in the principle of line of sight, so such typr of sensors can be utilised in the implementation. Implementing this prototype in real life would enable us make the train travel comfortable and precise. This system can be further upgraded to monitoring the train control remotely with an emergency remote control system for the worst case scenario. The facilities provided in the prototype is solely for the comfort and convenience of the passangers. This proposed system will lead to upgrade the train technology to a new level by taking optimum care of the passangers comfort, safety and punchuality.

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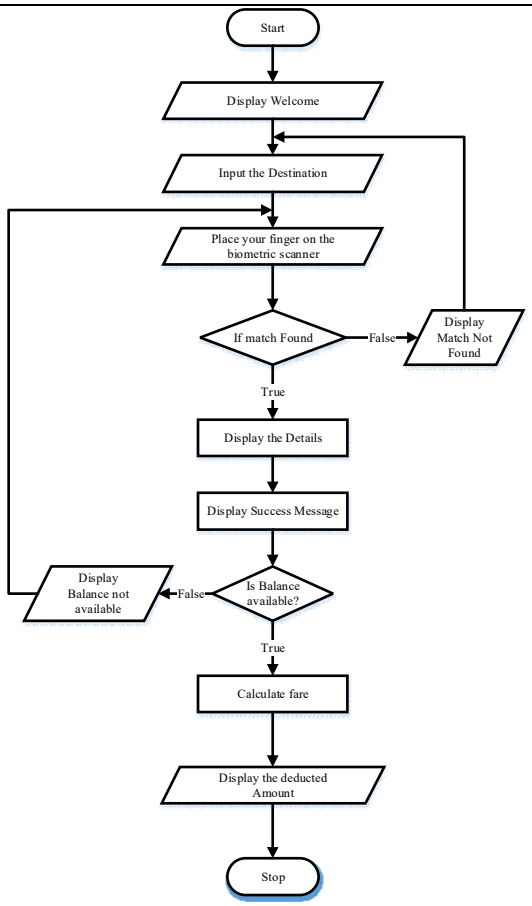

Fig 1: Flow Chart for Reservation system

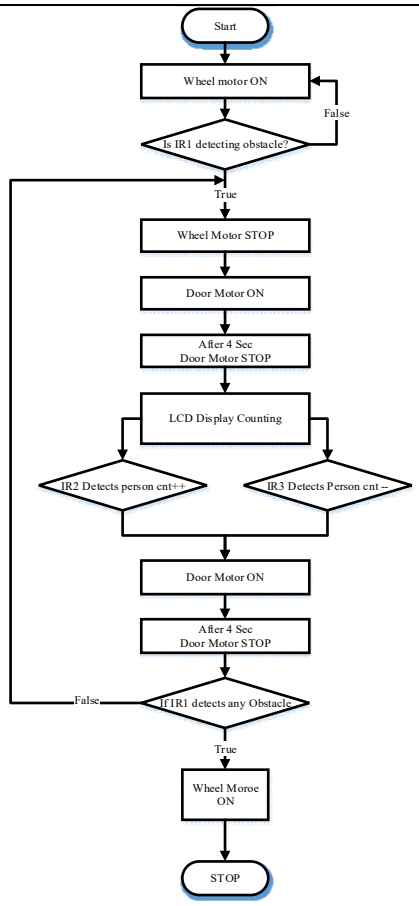

Fig2: Flow Chart for Automatic Metro System

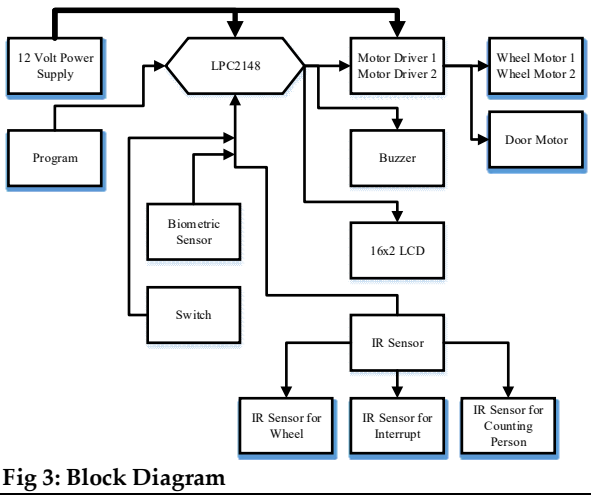

Fig 3: Block Diagram

Fig4: SFG Software

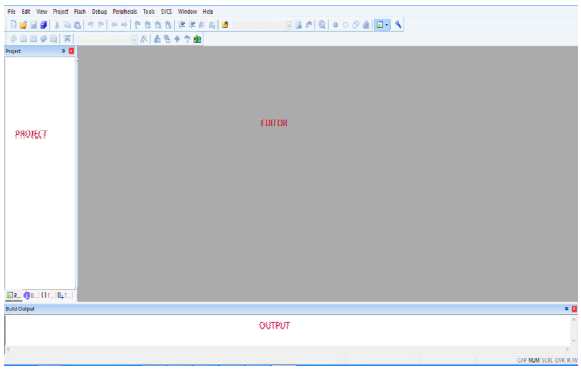

Fig 5: KeilµVision IDE

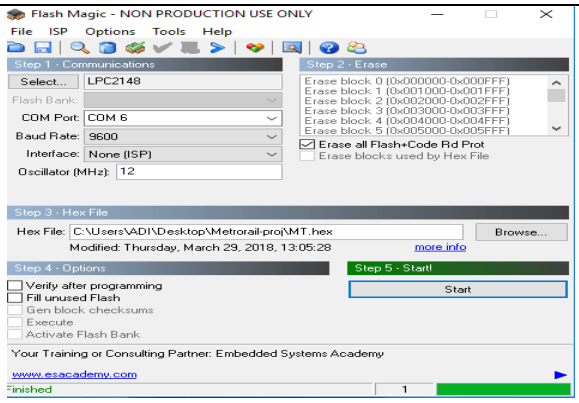

Fig 6: Flash magic

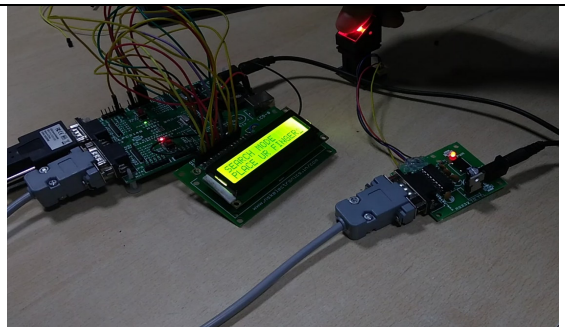

Fig7: Interfacing of Finger Print Sensor (R305) Module with LPC2148

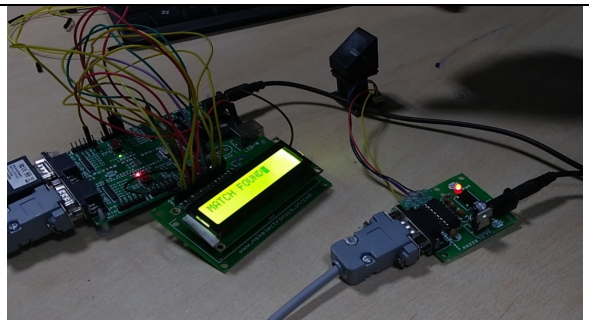

Fig 8. LCD Showing Successful Reservation

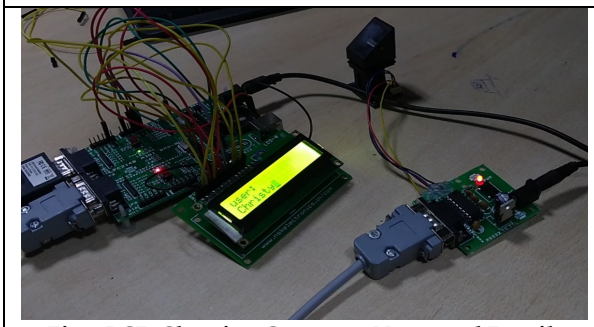

Fig9: LCD Showing Customer Name and Details

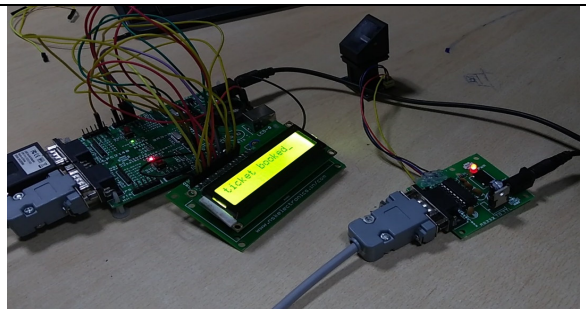

Fig10. LCD Displaying Successful Reservation of Ticket

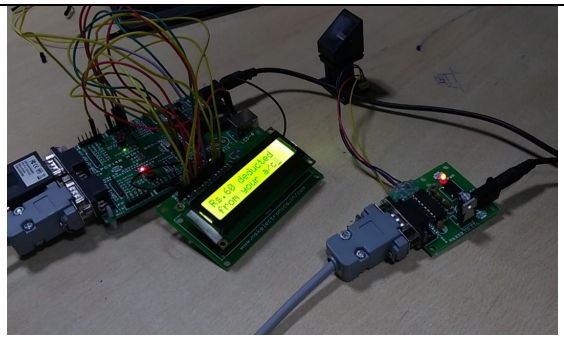

Fig 11: LCD Displaying the Travel Fare Details

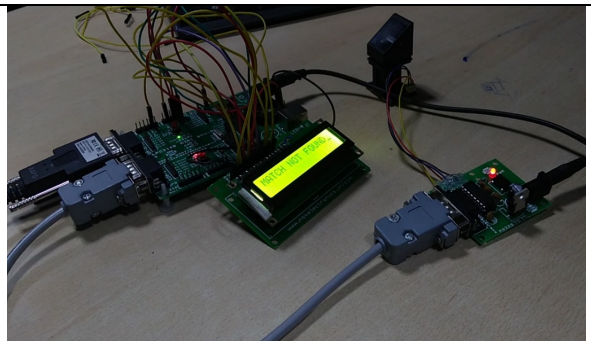

Fig.12: LCD Displaying Match not found

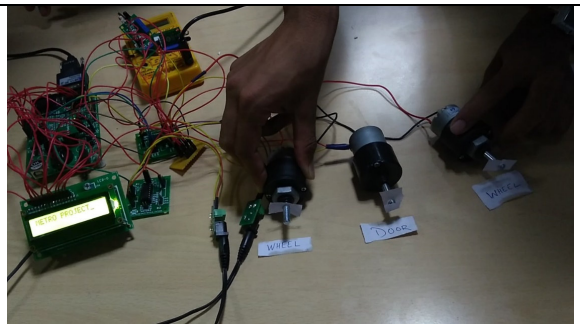

Fig.13. Initial Running Condition of the Metro Train

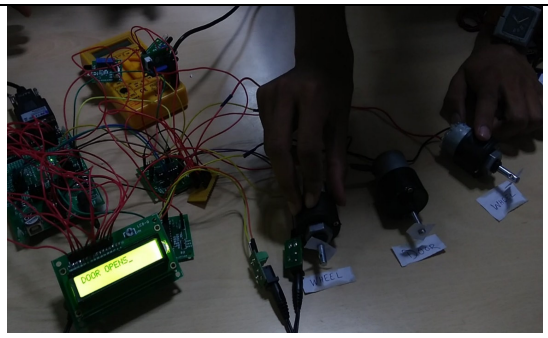

Fig.14: LCD Showing Successful Opening of Door

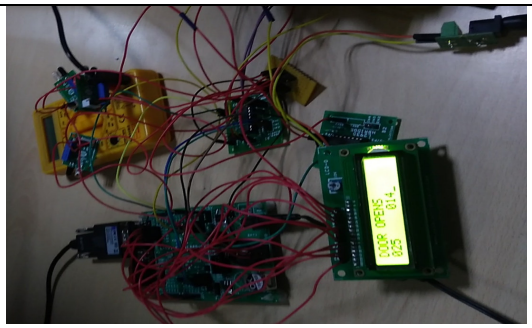

Fig 15: LCD Displaying Person Count

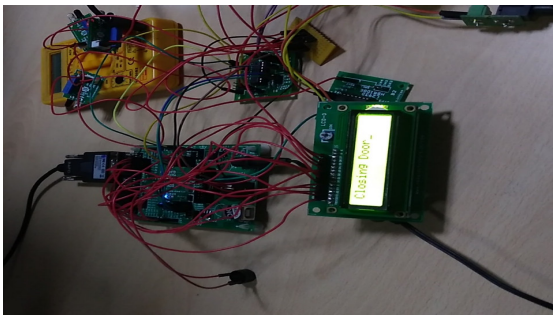

Fig 16: Successful Completion of the Person Count and Closing of the Door.

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RESEARCH ARTICLE

Vasicine May Inhibit the Activity of Free Enzyme of the 2019-nCoV Main Protease

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ABSTRACT

2019 Novel corona-virus (2019-nCoV) also referred to as severe acute respiratory syndrome Corona-virus 2 (SARS-CoV-2) emerged as a global risk and put the entire globe into unrest. Unavailability of specific drug against the virus is more imperative. *In silico* Molecular Docking revealed that the phytochemical, Vasicine effectively binds at the active pocket of the SARS-CoV-2 main protease.

Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, docking, phytochemicals, vasicine.

INTRODUCTION

The pandemic situation caused due to the 2019-nCoV represents a severe public health calamity across the globe. The city of Wuhan was the epicentre where the outbreak of this human pathogen emerged, and resulted to human ailment, termed as COVID-19 [1, 2]. 2019-nCoV encodes at least 27 proteins, including 15 non-structural proteins, 4 structural proteins, and 8 auxiliary proteins. SARS-CoV-2 belongs to the beta corona-virus genus, closely related to the previously identified severe acute respiratory syndrome corona-virus (SARS-CoV) [3, 4]. Public Health Emergency of International Concern (PHEIC) was declared by the World Health Organization (WHO) owing to its fast rate of transmission within the humans [1, 5, 6]. Crystal structure of the SARS-CoV-2 main protease (M^{pro}) proves to be an exceptional ground for screening specific ligands [7]. Reportedly, M^{pro} and other known viral proteins are defining features paving the path of virus from entry to infection in the host cell [8, 9, 10].

METHODS

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of M^{pro} was accessed from Protein Data Bank accession 6Y2E. The phytochemical, Vasicine was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking method [11] was used for molecular docking. The catalytic pocket of the M^{pro} protein was specified and targeted for binding of the ligand. CDOCKER Energy and CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the CDOCKER Energy, CDOCKER Interaction Energy and a diminutive difference between the CDOCKER Energy and CDOCKER Interaction Energy are considered to be the most favourable [12].

RESULTS AND DISCUSSION

It was found that vasicine; a common phytochemical specifically binds to the active pocket of the SARS-CoV-2 M^{pro} as apparent from higher CDOCKER energy and CDOCKER interaction energy (Table 1). Since, simple active bio molecule like Vasicine effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of Vasicine and eventually can be used in the pharmaceutical sector.

CONCLUSION AND FUTURE PERSPECTIVES

The current *in silico* molecular docking based study reveals that vasicine can target the reported SARS-CoV-2 M^{pro}. It would be extremely noteworthy being confirmed *in vivo*. It is crucial to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Phytochemicals like Vasicine is commercially available and thus may be effectively prescribed to circumvent the current global scenario. Essentially, this study makes an attempt to reveal simple phytochemicals like vasicine which can be employed for designing novel therapeutics.

Author contribution statement

GKP conceived the idea. GKP, SKS, PKP performed the experiments. All authors have significant contribution in drafting the manuscript.

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Ligand	Receptor			Interaction status	
Phytochemical	Protein	PDB Accession	Docking Result	CDocker Energy	CDocker Interaction Energy
Vasicine	Free Enzyme of the 2019-nCoV Main Protease	6Y2E	Positive	-8.91	-23.45

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RESEARCH ARTICLE

Vasicinone Binds to the Active Site of the Free Enzyme of the 2019-nCoV Main Protease

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RESULTS AND DISCUSSION

It was found that vasicinone; a common phytochemical specifically binds to the active pocket of the SARS-CoV-2 M^{pro} as apparent from higher CDOCKER energy and CDOCKER interaction energy (Table 1). Since, simple active bio molecule like Vasicinone effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of Vasicinone and eventually can be used in the pharmaceutical sector.

CONCLUSION AND FUTURE PERSPECTIVES

The current *in silico* molecular docking based study reveals that vasicinone can target the reported SARS-CoV-2 M^{pro}. It would be extremely noteworthy being confirmed *in vivo*. It is crucial to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Phytochemicals like vasicinone is commercially available and thus may be effectively prescribed to circumvent the current global scenario. Essentially, this study makes an attempt to reveal simple phytochemicals like vasicinone which can be employed for designing novel therapeutics.

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Ligand	Receptor			Interaction status	
Phytochemical	Protein	PDB Accession	Docking Result	CDocker Energy	CDocker Interaction Energy
Vasicinone	Free Enzyme of the 2019-nCoV Main Protease	6Y2E	Positive	-8.07	-22.87

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RESEARCH ARTICLE

Quercitin binds To the Free Enzyme of the 2019-nCoV Main Protease

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ABSTRACT

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Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, docking, phytochemicals, quercitin.

INTRODUCTION

The pandemic situation caused due to the 2019-nCoV represents a severe public health calamity across the globe. The city of Wuhan was the epicentre where the outbreak of this human pathogen emerged, and resulted to human ailment, termed as COVID-19 [1, 2]. 2019-nCoV encodes at least 27 proteins, including 15 non-structural proteins, 4 structural proteins, and 8 auxiliary proteins. SARS-CoV-2 belongs to the beta corona-virus genus, closely related to the previously identified severe acute respiratory syndrome corona-virus (SARS-CoV) [3, 4]. Public Health Emergency of International Concern (PHEIC) was declared by the World Health Organization (WHO) owing to its fast rate of transmission within the humans [1, 5, 6]. Crystal structure of the SARS-CoV-2 main protease (M^{pro}) proves to be an exceptional ground for screening specific ligands [7]. Reportedly, M^{pro} and other known viral proteins are defining features paving the path of virus from entry to infection in the host cell [8, 9, 10].

METHODS

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of M^{pro} was accessed from Protein Data Bank accession 6Y2E. The phytochemical, Quercitin was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

Molecular docking

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RESULTS AND DISCUSSION

It was found that quercitin; a common phytochemical specifically binds to the active pocket of the SARS-CoV-2 M^{pro} as apparent from higher CDOCKER energy and CDOCKER interaction energy (Table 1). Since, simple active bio molecule like Quercitin effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of Quercitin and eventually can be used in the pharmaceutical sector.

Conclusion and Future perspectives

The current *in silico* molecular docking based study reveals that quercitin can target the reported SARS-CoV-2 M^{pro}. It would be extremely noteworthy being confirmed *in vivo*. It is crucial to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Phytochemicals like quercitin is commercially available and thus may be effectively prescribed to circumvent the current global scenario. Essentially, this study makes an attempt to reveal simple phytochemicals like quercitin which can be employed for designing novel therapeutics.

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Phytochemical	Protein	PDB Accession	Docking Result	CDocker Energy	CDocker Interaction Energy
Quercitin	Free Enzyme of the 2019-nCoV Main Protease	6Y2E	Positive	-22.37	-29.64

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RESEARCH ARTICLE

Kaempferol May Bind To the Active Site of the Free Enzyme of the 2019-nCoV Main Protease

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Table 1: CDOCKER ENERGY and CDOCKER INTERACTION ENERGY values generated for the interaction of Kaempferol with the active site of SARS-CoV-2 main protease (M^{pro}).

Ligand	Receptor			Interaction status	
Phytochemical	Protein	PDB Accession	Docking Result	CDocker Energy	CDocker Interaction Energy
Kaempferol	Free Enzyme of the 2019-nCoV Main Protease	6Y2E	Positive	-18.58	-21.81

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RESEARCH ARTICLE

Aloeemodin May Deactivate the Free Enzyme of the 2019-nCoV Main Protease

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ABSTRACT

2019 Novel corona-virus (2019-nCoV) also referred to as severe acute respiratory syndrome Corona-virus 2 (SARS-CoV-2) emerged as a global risk and put the entire globe into unrest. Unavailability of specific drug against the virus is more imperative. *In silico* Molecular Docking revealed that the phytochemical, Aloeemodin effectively binds at the active pocket of the SARS-CoV-2 main protease.

Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, docking, phytochemicals, Aloeemodin

INTRODUCTION

The pandemic situation caused due to the 2019-nCoV represents a severe public health calamity across the globe. The city of Wuhan was the epicentre where the outbreak of this human pathogen emerged, and resulted to human ailment, termed as COVID-19 [1, 2]. 2019-nCoV encodes at least 27 proteins, including 15 non-structural proteins, 4 structural proteins, and 8 auxiliary proteins. SARS-CoV-2 belongs to the beta corona-virus genus, closely related to the previously identified severe acute respiratory syndrome corona-virus (SARS-CoV) [3, 4]. Public Health Emergency of International Concern (PHEIC) was declared by the World Health Organization (WHO) owing to its fast rate of transmission within the humans [1, 5, 6]. Crystal structure of the SARS-CoV-2 main protease (M^{pro}) proves to be an exceptional ground for screening specific ligands [7]. Reportedly, M^{pro} and other known viral proteins are defining features paving the path of virus from entry to infection in the host cell [8, 9, 10].

METHODS

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of M^{pro} was accessed from Protein Data Bank accession 6Y2E. The phytochemical, Aloeemodin was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking method [11] was used for molecular docking. The catalytic pocket of the M^{pro} protein was specified and targeted for binding of the ligand. CDOCKER Energy and CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the CDOCKER Energy, CDOCKER Interaction Energy and a diminutive difference between the CDOCKER Energy and CDOCKER Interaction Energy are considered to be the most favourable [12].

RESULTS AND DISCUSSION

It was found that Aloeemodin ; a common phytochemical specifically binds to the active pocket of the SARS-CoV-2 M^{pro} as apparent from higher CDOCKER energy and CDOCKER interaction energy (Table 1). Since, simple active bio molecule like Aloeemodin effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of Aloeemodin and eventually can be used in the pharmaceutical sector.

CONCLUSION AND FUTURE PERSPECTIVES

The current *in silico* molecular docking based study reveals that Aloeemodin can target the reported SARS-CoV-2 M^{pro}. It would be extremely noteworthy being confirmed *in vivo*. It is crucial to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Phytochemicals like Aloeemodin is commercially available and thus may be effectively prescribed to circumvent the current global scenario. Essentially, this study makes an attempt to reveal simple phytochemicals like Aloeemodin which can be employed for designing novel therapeutics.

Author contribution statement

GKP conceived the idea. GKP, SKS, PKP performed the experiments. All authors have significant contribution in drafting the manuscript.

Funding

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Conflict of interest

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Table 1: CDOCKER ENERGY and CDOCKER INTERACTION ENERGY values generated for the interaction of Aloeemodin with the active site of SARS-CoV-2 main protease (M^{pro}).

Ligand	Receptor			Interaction status	
Phytochemical	Protein	PDB Accession	Docking Result	CDocker Energy	CDocker Interaction Energy
Aloeemodin	Free Enzyme of the 2019-nCoV Main Protease	6Y2E	Positive	-18.07	-23.27

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RESEARCH ARTICLE

Bufotenine May Bind To the Active Site of the Free Enzyme of the 2019-nCoV Main Protease

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ABSTRACT

2019 Novel corona-virus (2019-nCoV) also referred to as severe acute respiratory syndrome Corona-virus 2 (SARS-CoV-2) emerged as a global risk and put the entire globe into unrest. Unavailability of specific drug against the virus is more imperative. *In silico* Molecular Docking revealed that the phytochemical, Bufotenine effectively binds at the active pocket of the SARS-CoV-2 main protease.

Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, docking, phytochemicals, Bufotenine.

INTRODUCTION

The pandemic situation caused due to the 2019-nCoV represents a severe public health calamity across the globe. The city of Wuhan was the epicentre where the outbreak of this human pathogen emerged, and resulted to human ailment, termed as COVID-19 [1, 2]. 2019-nCoV encodes at least 27 proteins, including 15 non-structural proteins, 4 structural proteins, and 8 auxiliary proteins. SARS-CoV-2 belongs to the beta corona-virus genus, closely related to the previously identified severe acute respiratory syndrome corona-virus (SARS-CoV) [3, 4]. Public Health Emergency of International Concern (PHEIC) was declared by the World Health Organization (WHO) owing to its fast rate of transmission within the humans [1, 5, 6]. Crystal structure of the SARS-CoV-2 main protease (M^{pro}) proves to be an exceptional ground for screening specific ligands [7]. Reportedly, M^{pro} and other known viral proteins are defining features paving the path of virus from entry to infection in the host cell [8, 9, 10].

METHODS

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of M^{pro} was accessed from Protein Data Bank accession 6Y2E. The phytochemical, Bufotenine was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking method [11] was used for molecular docking. The catalytic pocket of the M^{pro} protein was specified and targeted for binding of the ligand. CDOCKER Energy and CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the CDOCKER Energy, CDOCKER Interaction Energy and a diminutive difference between the CDOCKER Energy and CDOCKER Interaction Energy are considered to be the most favourable [12].

RESULTS AND DISCUSSION

It was found that Bufotenine; a common phytochemical specifically binds to the active pocket of the SARS-CoV-2 M^{pro} as apparent from higher CDOCKER energy and CDOCKER interaction energy (Table 1). Since, simple active bio molecule like Bufotenine effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of Bufotenine and eventually can be used in the pharmaceutical sector.

CONCLUSION AND FUTURE PERSPECTIVES

The current *in silico* molecular docking based study reveals that Bufotenine can target the reported SARS-CoV-2 M^{pro}. It would be extremely noteworthy being confirmed *in vivo*. It is crucial to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Phytochemicals like Bufotenine is commercially available and thus may be effectively prescribed to circumvent the current global scenario. Essentially, this study makes an attempt to reveal simple phytochemicals like Bufotenine which can be employed for designing novel therapeutics.

Author contribution statement

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Conflict of interest

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Table 1: CDOCKER ENERGY and CDOCKER INTERACTION ENERGY values generated for the interaction of Bufotenine with the active site of SARS-CoV-2 main protease (M^{pro}).

Ligand	Receptor			Interaction status	
Phytochemical	Protein	PDB Accession	Docking Result	CDocker Energy	CDocker Interaction Energy
Bufotenine	Free Enzyme of the 2019-nCoV Main Protease	6Y2E	Positive	-12.97	-18.64

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RESEARCH ARTICLE

Dopamine Interacts with the Free Enzyme of the 2019-nCoV Main Protease

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ABSTRACT

2019 Novel corona-virus (2019-nCoV) also referred to as severe acute respiratory syndrome Corona-virus 2 (SARS-CoV-2) emerged as a global risk and put the entire globe into unrest. Unavailability of specific drug against the virus is more imperative. *In silico* Molecular Docking revealed that the phytochemical, Dopamine effectively binds at the active pocket of the SARS-CoV-2 main protease.

Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, docking, phytochemicals, Dopamine.

INTRODUCTION

The pandemic situation caused due to the 2019-nCoV represents a severe public health calamity across the globe. The city of Wuhan was the epicentre where the outbreak of this human pathogen emerged, and resulted to human ailment, termed as COVID-19 [1, 2]. 2019-nCoV encodes at least 27 proteins, including 15 non-structural proteins, 4 structural proteins, and 8 auxiliary proteins. SARS-CoV-2 belongs to the beta corona-virus genus, closely related to the previously identified severe acute respiratory syndrome corona-virus (SARS-CoV) [3, 4]. Public Health Emergency of International Concern (PHEIC) was declared by the World Health Organization (WHO) owing to its fast rate of transmission within the humans [1, 5, 6]. Crystal structure of the SARS-CoV-2 main protease (M^{pro}) proves to be an exceptional ground for screening specific ligands [7]. Reportedly, M^{pro} and other known viral proteins are defining features paving the path of virus from entry to infection in the host cell [8, 9, 10].

METHODS

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of M^{pro} was accessed from Protein Data Bank accession 6Y2E. The phytochemical, Dopamine was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking method [11] was used for molecular docking. The catalytic pocket of the M^{pro} protein was specified and targeted for binding of the ligand. CDOCKER Energy and CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the CDOCKER Energy, CDOCKER Interaction Energy and a diminutive difference between the CDOCKER Energy and CDOCKER Interaction Energy are considered to be the most favourable [12].

RESULTS AND DISCUSSION

It was found that Dopamine; a common phytochemical specifically binds to the active pocket of the SARS-CoV-2 M^{pro} as apparent from higher CDOCKER energy and CDOCKER interaction energy (Table 1). Since, simple active bio molecule like Dopamine effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of Dopamine and eventually can be used in the pharmaceutical sector.

CONCLUSION AND FUTURE PERSPECTIVES

The current *in silico* molecular docking based study reveals that Dopamine can target the reported SARS-CoV-2 M^{pro}. It would be extremely noteworthy being confirmed *in vivo*. It is crucial to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Phytochemicals like Dopamine is commercially available and thus may be effectively prescribed to circumvent the current global scenario. Essentially, this study makes an attempt to reveal simple phytochemicals like Dopamine which can be employed for designing novel therapeutics.

Author contribution statement

GKP conceived the idea. GKP, SKS, PKP performed the experiments. All authors have significant contribution in drafting the manuscript.

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Table 1: CDOCKER ENERGY and CDOCKER INTERACTION ENERGY values generated for the interaction of Dopamine with the active site of SARS-CoV-2 main protease (M^{pro}).

Ligand	Receptor			Interaction status	
Phytochemical	Protein	PDB Accession	Docking Result	CDocker Energy	CDocker Interaction Energy
Dopamine	Free Enzyme of the 2019-nCoV Main Protease	6Y2E	Positive	-11.32	-14.58

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RESEARCH ARTICLE

Quercitin May Stall the Activity of Papain-like Protease of SARS-CoV-2

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ABSTRACT

2019 Novel corona-virus (2019-nCoV) also referred to as severe acute respiratory syndrome Corona-virus 2 (SARS-CoV-2) emerged as a global risk and put the entire globe into unrest. Unavailability of specific drug against the virus is more imperative. *In silico* Molecular Docking revealed that the phytochemical, Quercitin effectively binds at the active pocket of the SARS-CoV-2 main protease.

Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, docking, phytochemicals, Quercitin.

INTRODUCTION

The pandemic situation caused due to the 2019-nCoV represents a severe public health calamity across the globe. The city of Wuhan was the epicentre where the outbreak of this human pathogen emerged, and resulted to human ailment, termed as COVID-19 [1, 2]. 2019-nCoV encodes at least 27 proteins, including 15 non-structural proteins, 4 structural proteins, and 8 auxiliary proteins. SARS-CoV-2 belongs to the beta corona-virus genus, closely related to the previously identified severe acute respiratory syndrome corona-virus (SARS-CoV) [3, 4]. Public Health Emergency of International Concern (PHEIC) was declared by the World Health Organization (WHO) owing to its fast rate of transmission within the humans [1, 5, 6]. Crystal structure of the Papain-like Protease of SARS-CoV-2 proves to be an exceptional ground for screening specific ligands [7]. Reportedly, M^{pro} and other known viral proteins are defining features paving the path of virus from entry to infection in the host cell [8, 9, 10].

METHODS

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of Papain-like Protease of SARS-CoV-2 was accessed from Protein Data Bank accession 6W9C. The phytochemical, Quercitin was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking method [11] was used for molecular docking. The catalytic pocket of the Papain-like Protease of SARS-CoV-2 was specified and targeted for binding of the ligand. CDOCKER Energy and CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the CDOCKER Energy, CDOCKER Interaction Energy and a diminutive difference between the CDOCKER Energy and CDOCKER Interaction Energy are considered to be the most favourable [12].

RESULTS AND DISCUSSION

It was found that Quercitin; a common phytochemical specifically binds to the active pocket of the Papain-like Protease of SARS-CoV-2 as apparent from higher CDOCKER energy and CDOCKER interaction energy (Table 1). Since, simple active bio molecule like Quercitin effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of Quercitin and eventually can be used in the pharmaceutical sector.

CONCLUSION AND FUTURE PERSPECTIVES

The current *in silico* molecular docking based study reveals that Quercitin can target the reported Papain-like Protease of SARS-CoV-2. It would be extremely noteworthy being confirmed *in vivo*. It is crucial to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Phytochemicals like Quercitin is commercially available and thus may be effectively prescribed to circumvent the current global scenario. Essentially, this study makes an attempt to reveal simple phytochemicals like Quercitin which can be employed for designing novel therapeutics.

Author contribution statement

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Table 1: CDOCKER ENERGY and CDOCKER INTERACTION ENERGY values generated for the interaction of Quercitin with the active site of Papain-like Protease of SARS-CoV-2.

Ligand	Receptor			Interaction status	
Phytochemical	Protein	PDB Accession	Docking Result	CDocker Energy	CDocker Interaction Energy
Quercitin	Papain-like Protease of SARS-CoV-2	6W9C	Positive	-27.89	-29.67

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RESEARCH ARTICLE

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Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, docking, phytochemicals, Kaempferol.

INTRODUCTION

The pandemic situation caused due to the 2019-nCoV represents a severe public health calamity across the globe. The city of Wuhan was the epicentre where the outbreak of this human pathogen emerged, and resulted to human ailment, termed as COVID-19 [1, 2]. 2019-nCoV encodes at least 27 proteins, including 15 non-structural proteins, 4 structural proteins, and 8 auxiliary proteins. SARS-CoV-2 belongs to the beta corona-virus genus, closely related to the previously identified severe acute respiratory syndrome corona-virus (SARS-CoV) [3, 4]. Public Health Emergency of International Concern (PHEIC) was declared by the World Health Organization (WHO) owing to its fast rate of transmission within the humans [1, 5, 6]. Crystal structure of the Papain-like Protease of SARS-CoV-2 proves to be an exceptional ground for screening specific ligands [7]. Reportedly, M^{pro} and other known viral proteins are defining features paving the path of virus from entry to infection in the host cell [8, 9, 10].

METHODS

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of Papain-like Protease of SARS-CoV-2 was accessed from Protein Data Bank accession 6W9C. The phytochemical, Kaempferol was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking method [11] was used for molecular docking. The catalytic pocket of the Papain-like Protease of SARS-CoV-2 was specified and targeted for binding of the ligand. CDOCKER Energy and CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the CDOCKER Energy, CDOCKER Interaction Energy and a diminutive difference between the CDOCKER Energy and CDOCKER Interaction Energy are considered to be the most favourable [12].

RESULTS AND DISCUSSION

It was found that Kaempferol; a common phytochemical specifically binds to the active pocket of the Papain-like Protease of SARS-CoV-2 as apparent from higher CDOCKER energy and CDOCKER interaction energy (Table 1). Since, simple active bio molecule like Kaempferol effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of Kaempferol and eventually can be used in the pharmaceutical sector.

CONCLUSION AND FUTURE PERSPECTIVES

The current *in silico* molecular docking based study reveals that Kaempferol can target the reported Papain-like Protease of SARS-CoV-2. It would be extremely noteworthy being confirmed *in vivo*. It is crucial to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Phytochemicals like Kaempferol is commercially available and thus may be effectively prescribed to circumvent the current global scenario. Essentially, this study makes an attempt to reveal simple phytochemicals like Kaempferol which can be employed for designing novel therapeutics.

Author contribution statement

GKP conceived the idea. GKP, SKS, PKP performed the experiments. All authors have significant contribution in drafting the manuscript.

Funding

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Conflict of interest

The authors declare that they have no conflict of interest.

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Table 1: CDOCKER ENERGY and CDOCKER INTERACTION ENERGY values generated for the interaction of Kaempferol with the active site of Papain-like Protease of SARS-CoV-2.

Ligand	Receptor			Interaction status	
Phytochemical	Protein	PDB Accession	Docking Result	CDocker Energy	CDocker Interaction Energy
Kaempferol	Papain-like Protease of SARS-CoV-2	6W9C	Positive	-24.68	-29.31

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RESEARCH ARTICLE

Aloeemodin Inhibits the Activity of Papain-like Protease of SARS-CoV-2

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ABSTRACT

2019 Novel corona-virus (2019-nCoV) also referred to as severe acute respiratory syndrome Corona-virus 2 (SARS-CoV-2) emerged as a global risk and put the entire globe into unrest. Unavailability of specific drug against the virus is more imperative. *In silico* Molecular Docking revealed that the phytochemical, Aloeemodin effectively binds at the active pocket of the SARS-CoV-2 main protease.

Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, docking, phytochemicals, Aloeemodin.

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