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Prediction of Permeability for a composite of tetmeth bisphen carbonate and nylon6

Rabindra Singh¹, Dr Santosh Satapathy²

¹180705120005@cutm.ac.in, ²santosh.satpathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of tetmeth_bisphen_carbonate and nylon6. Synthia module of Biovia Materials Studio software was used to predict Glass transition temperature, Density, Oxygen permeability, Nitrogen permeability and Carbon dioxide permeability of the composite.

Objective: In this study the effect of mixing of tetmeth_bisphen_carbonate and nylon6 on the following properties have been predicted.

- a. Glass transition temperature
- b. Density
- c. Oxygen permeability
- d. Nitrogen permeability
- e. Carbon dioxide permeability

The weight fractions of the monomers were varied in the range of 0 to 1.

Software used: Synthia module of Biovia Materials Studio software (Dassault Systemes, France) was used for the study.

Results and Discussion: The effect of weight fraction of tetmeth_bisphen_carbonate (Monomer 1) on the Permeability of the composite has been presented in Table 1. The predicted properties of the composite for 0, 0.5 and 1.0 weight fractions of tetmeth_bisphen_carbonate have been summarized in Table 1. The rate of change for the properties have been summarized in Table 2.

Table 1. Properties of composite of tetmeth_bisphen_carbonate and nylon6

| Property | | Results for | | |
|--|-----------|------------------------|------------------------|------------------------|
| Name | Uni | 0.0 weight fraction of | 0.5 weight fraction of | 1.0 weight fraction of |
| | t | tetmeth_bisphen_carbo | tetmeth_bisphen_carbo | tetmeth_bisphen_carbo |
| | | nate | nate | nate |
| Glass transition temperatur e | oC | 328.410 | 398.978 | 466.509 |
| Density | kg per | 1.078 | 1.079 | 1.080 |

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