Prediction of Permeability for a composite of bisphen_dimeth_carbonate and acrylonitrile

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of bisphen_dimeth_carbonate and acrylonitrile. 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 bisphen_dimeth_carbonate and acrylonitrile 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 bisphen_dimeth_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 bisphen_dimeth_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 bisphen_dimeth_carbonate and acrylonitrile

Property		Results for		
Name	Unit	0.0 weight fraction of bisphen_dimeth_carbonate	0.5 weight fraction of bisphen_dimeth_carbonate	1.0 weight fraction of bisphen_dimeth_carbonate
Glass transition temperature	oC	361.527	388.227	414.398
Density	kg per	1.177	1.176	1.174