

Prediction of Permeability for a composite of bisphen_dimeth_carbonate and benzamide

Anubhaba Mohapatra¹, Mr. Shraban Kumar Sahoo²

¹180705100008@cutm.ac.in, ²shraban.sahoo@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 bisphen_dimeth_carbonate and benzamide. 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 benzamide 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 benzamide

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	603.481	510.692	414.398
Density	kg per	1.295	1.232	1.174