Prediction of Permeability for a composite of tetmeth_bisphen_carbonate and vinyl_acetate

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Abstract: A computational study has been done to predict Permeability of a polymer composite consisting of tetmeth_bisphen_carbonate and vinyl_acetate. 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 vinyl_acetate 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 vinyl_acetate

Property		Results for		
Name	Unit	0.0 weight fraction of tetmeth_bisphen_carbonate	0.5 weight fraction of tetmeth_bisphen_carbonate	1.0 weight fraction of tetmeth_bisphen_carbonate
Glass transition temperature	oC	302.653	386.461	466.509
Density	kg per	1.219	1.145	1.080

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