NANOPORE-LEVEL MODELING OF THE TRANSPORT OF WATER AND OXYGEN IN POLYMERIC FILMS

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Abstract. Results for simulations of the transport of water vapor, oxygen and liquid water in polymeric films at pore level are presented. Two kinds of mechanisms are considered: transport of oxygen and water vapor in the gas phase and transport of liquid water. The model is based on physical aspects of the condensation process and the morphology and connectivity of the porous medium. The objective of this work is to present a 3D nanopore scale model for the transport of liquid water, water vapor and oxygen in polymeric films. The porous media is represented by a three-dimensional cubic network with pore segments randomly assigned according to a Log-normal distribution function and the model is solved using the Monte Carlo method. As water vapor flows into the polymeric film, condensation of water occurs at the pore walls of the network. Liquid in pore corners allows hydraulic connectivity throughout the network at all time and capillary pressure is determined by modified Young-Laplace equation. The transport of water vapor and oxygen are modeled using the Ficks equation and the transport of the liquid water is determined using the Darcys law. With Monte Carlo sampling we find optimum network size in 3D to avoid size effects (40x20x40). Here we report pore-level distribution of liquid and vapor as transport phenomena advanced, effective water vapor, liquid and oxygen diffusivity and absolute permeability are calculated and the results correspond to a mean value of 10 repetitions. The transport properties obtained by the model are compared with experimental results obtained by specialized literature and a good agreement for the oxygen and water vapor was achieved.

Keywords: Condensation; diffusivity; pore-level; oxygen; water vapor; liquid water.

Mathematics Subject Classifications (2000): 34F05.

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