NANOPORE SCALE MODEL FOR THE TRANSPORT OF LIQUID WATER, WATER VAPOR AND OXYGEN IN POLYMERIC FILMS. APPLICATIONS TO FOOD PACKING.

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The mass transport control through the packaging film is extremely important to guarantee the proper shelf-life of the packaged products. Then a better knowledge of the factors that governing the transport properties is required to improve the phenomenon comprehension. 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 polymer considered as a nanoporous media is represented by a three-dimensional cubic network with nanopore segments randomly assigned and the model is solved using Monte Carlo method. As water vapor flows into the polymeric film, condensation of water occurs at the nanopore walls of the network. Liquid in nanopore corners allows hydraulic connectivity throughout the network at all time and capillary pressure is determined by augmented Young-Laplace equation. Here we report pore-level distribution of liquid and vapor and capillary pressure as transport phenomena advanced, effective water vapor, liquid vapor and oxygen diffusivity and absolute permeability are calculated. The vapor and oxygen diffusivity diminish as vapor condensation occurs from $9.54 \times 10^{-8}$ to $3.77 \times 10^{-10}$ [cm$^2$/s] and $8.33 \times 10^{-8}$ to $3.25 \times 10^{-10}$ [cm$^2$/s] respectively. The vapor and oxygen permeability diminish from $1.17 \times 10^{-21}$ to $1.10 \times 10^{-24}$ [m$^2$] and $3.35 \times 10^{-21}$ to $3.13 \times 10^{-24}$ [m$^2$]. On the other hand, the hydraulic permeability increases from $2.64 \times 10^{-25}$ to $7.06 \times 10^{-21}$ [m$^2$]. The transport properties obtained by the model were compared with experimental results obtained by specialized literature given a good agreement for the oxygen and water vapor. Finally, the transport model for water vapor and oxygen developed is applicable to food polymeric films intended for food packing applications.

Keywords: condensation; diffusivity; pore-level; oxygen; water vapor

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