

A SIMPLE 2D PORE-SCALE NETWORK MODEL FOR THE TRANSPORT OF WATER VAPOR AND OXYGEN IN POLYMERIC FILMS

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Abstract— A mathematical model was developed to describe mass transport in polymeric films based on modifications of Fick's law in a continuous macroscopic approach. The purpose of this work was specifically to model the transport of water vapor and oxygen in polymeric films at the pore level, based on physical aspects of the condensation process and the morphology and connectivity of the porous medium, with two-dimensional pore networks representing pore spaces. Using a Pore scale discrete model, we found that the pore-level distributions of liquid (condensate) and vapor as transport phenomena occurred. The vapor and oxygen diffusivities ranged from 4.22×10^{-6} to 3.16×10^{-7} cm²/s and from 3.66×10^{-6} to 2.86×10^{-7} cm²/s, respectively. Also, the vapor and oxygen permeabilities ranged from 2.61×10^{-3} to 3.83×10^{-4} nD ($1 \text{ nD} = 10^{-21} \text{ m}^2$) and from 6.77×10^{-3} to 1.35×10^{-3} nD, respectively. The transport properties obtained by the model were compared with the corresponding results for chitosan films obtained in previous experimental studies, showing a partial agreement.

Keywords— condensation, diffusivity, porous film, oxygen, water vapor

I. INTRODUCTION

Polymers have been commonly used for food packaging due to their characteristics such as versatility in the manufacturing of different packages, low cost, light weight and chemical inertness (Del-Valle *et al.*, 2003). It is well known that polymeric films can control the transport of low-molecular-weight compounds through the packaging, thus preserving the packaged foods during storage (Del Nobile *et al.*, 2003a, 2003b). The barrier properties of flexible films can be measured by the use of permeability and diffusivity coefficients (water vapor or gas). These are intensive macroscopic properties that represent the overall resistance of the films offer to the passage of gas fluid (water vapor or oxygen).

The classical macroscopic mathematical models developed to describe the transport of water vapor and gases through polymeric films have been described in terms of the solubilization-diffusion mechanism, governed by both thermodynamic and kinetic factors (Hernandez, 1994; Del Nobile *et al.*, 2003a, 2003b, 2004). There is another approach to solving this problem, the microscopic models. These kinds of models are based on the transport properties and physical characteristics of the film at the pore-level scale such as: wettability in function of the contact angle, pore size distribution (a

measure of the porosity, pores size), pore geometry (a measure of the pore shape cross-section, circular, polygonal, etc.), and topology (connectivity between the pores). The traditional mathematical models used to explain the mass transfer in polymeric films do not make difference between the two main mechanisms of mass transfer (in gas phase and in liquid phase), i.e., the models are based on Fick's law modifications with and adjust parameter variable on time. On the other hand, those kinds of models do not able to show the liquid distribution as condensation occurs during the process. The percolation model has enough skills to model the condensation in-situ, because it is possible to simulate the liquid quantity that residing into the nanopores walls in function of the morphology and topology of the porous structure and also it is possible to simulate the process evolution on the time. Pore-level models have not yet been used to model the transport phenomena at the nanopore-scale but they have been used to model water-vapor condensation and transport phenomena at the micropore-scale, mainly in oil reservoirs (Mohammadi *et al.*, 1990; Fang *et al.*, 1996; Li and Firozabaadi, 2000; Bustos and Toledo, 2003a, 2003b).

An important phenomenon that occurs at the pore level when a gas phase is present is in-situ condensation. When the total pressure in a porous media goes down condensation occurs and this phenomenon is named retrograde condensation. At the beginning of the condensation the gas effective permeability or diffusivity remains high, but as total pressure decreases condensate tends to fill more space within pore structure diminishing the transport properties in the gas phase (gas permeability or gas diffusivity). Once the critical condensation is reached, the transport phenomena in the gas phase become zero (Bustos and Toledo, 2003a). How abruptly it decreases depends on the pore structure, fluid properties and operating conditions. Bustos and Toledo (2003a, 2003b) studied the effects of contact-angle hysteresis, pore-size distribution and pore shape on the relative permeability of gas and condensate in two- and three-dimensional pore networks at the micropore-scale.

The objective of this work was to present a nanopore-level model of the transport of water vapor and oxygen applicable to polymeric films. We consider that the polymer is theoretically a system compose of impermeable matter through which co-exist interconnected pores (nanopores) where the diffusion mechanisms could occur. A two-dimensional network model was selected to represent the pore space and the model was solved using a Monte Carlo method based on a pre-