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3D modelling of gas permeation through composite PVA/TiO_2 and PVA/MMT thin films

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Extended Abstract

Polyvinyl alcohol (PVA) films, a polymer with excellent mechanical, biodegradable and water-soluble properties, have been widely studied and proposed for numerous applications, such as controlled release in pharmaceutical elements, fuel cells, solar cells, and batteries. Furthermore, the barrier properties of PVA toward oxygen and carbon dioxide have led to its application in food packaging [1, 2]. Different studies have shown that titanium oxide (TiO_2) or/and Montmorillonite (MMT) nanoclay as filler particles enhance barrier and mechanical properties of the composite membranes, compared to pure PVA membranes [3, 4]. MMT nanoclay particles, especially, with a generally high aspect ratio, helps in forming thin barrier films. The aspect ratio, volume fraction, and the orientation angle of the nanoparticles within the polymer are important factors that determine the effective gas permeability of the films for specific gases.

In this project, MMT nanoclay (thickness = 1-2 nm), TiO_2 (diameter = 20 nm), and PVA (MW = 145000 g/mol) were used to prepare solutions. The nanocomposite membranes were made using three different methods: solvent casting, spraying, and spin coating. The membranes were then tested in a standard constant-volume gas permeation system, described elsewhere [5]. As a result, the permeability and diffusivity were evaluated by monitoring the pressure rise at the permeate side of the membrane. The permeation process was then numerically simulated with a 3D numerical model using finite differences to predict the gas permeation and diffusion behaviours of the composites membranes.

In the simulations, the nanoparticles were assumed impermeable, the geometry of TiO_2 was assumed spherical, and the geometry of MMT nanoclay was assumed to be well represented by thin parallelepipeds. Single particles laying horizontally within a PVA polymer membrane were first studied to understand the effect of the geometries on the composite membrane's effective permeability. A series of simulations were then performed to study the permeation with nanofiller particles were subjected to three-dimensional rotations. Eventually, the effect of particle volume fraction ϕ was tested. The results show that different angles of filler particle orientation play a critical role in gas effective permeability of the membranes.

References

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