

4ci Mass Transport through Polymer: from Theoretic to Experimental

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Mass transport of small molecules through polymeric materials occurs in many applications, such as in gas separation, protective clothing, packaging, coating, drug delivery, etc. Many factors can influence the mass transport process, such as temperature, the nature of the polymer, external mechanical deformations, etc. My research interest has been focus on how the external mechanical deformation and the internal structure of polymer can change the mass transport process.

Theoretic: Fick's laws are normally used to describe the mass transport process. However, due to the polymer's visco-elastic properties, the mass transport process of small molecules transport through polymeric materials is very complex and cannot be expressed fully by Fick's laws. During my PhD study at Tulane University (Advisor: Daniel De Kee), I used two different approaches to developed a mathematic model to describe non-Fickian process. Those models modify Fick's laws and describe convective fluxes due to the polymer viscoelasticity and/or the complex interfaces in a polymer based composites. The first mesoscopic method makes use of the Hamiltonian/bracket and GENERIC formalisms and create two parameters account for the effect of the polymer viscoelasticity and two for the complex interfaces influence. Another continuum mechanics approach includes a convective flux due to the stress. Both models yield quantitative agreement with the experimental data and provide an indication of whether the transport process is Fickian or non-Fickian.

Experimental: Polymer based nanocomposites show improved mechanical, thermal, as well as barrier properties. During my PhD study, I build an experimental setup to test the permeation of solvent through PDMS/montmorillonite nanocomposite under uni- or biaxial mechanical deformation. The extension of the membrane not only decrease the thickness of the membrane, which enhances the diffusion process, but also pack the polymer chains (decreasing the free volume), which decreases the diffusion coefficient. My current Post-doc research (with Professor Edward Cussler) is to test the flake-filled barrier membrane made by photo lithography. Barrier membranes with carefully patterned metal flakes have been prepared by means of photo lithography. The shape, aspect ratio and volume ratio of the metal flake are varied. The flakes are typically 100 micron square and 1 micron thick, present at volume fractions of 0.10. Gas permeation experiments carried out using these composite barriers show permeability reductions which are over two orders of magnitude. Complementally mechanical measurements show how these permeability reductions are gained at a cost of poorer flexibility and toughness. These permeability and mechanical measurements are compared with available theories to discover how films with low permeability and high flexibility can be made.