

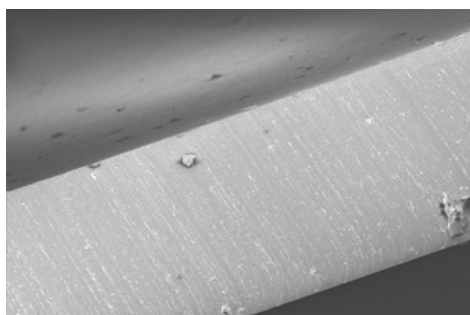
Small Molecule Diffusion Through Nanoscale Systems

Lupita Bermudez, Donna Phu, Heather Schalliol, Christina Tang, and Nancy Lape

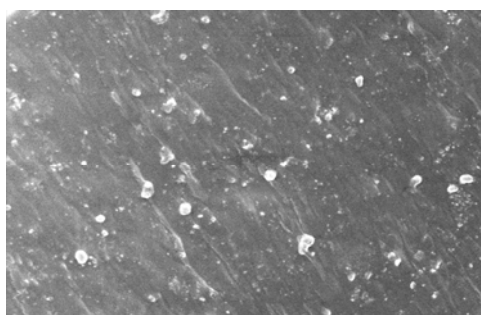
Background. Recent research has found that the addition of inorganic nanoparticles to ultra-high free volume glassy polymers increases membrane gas permeability with no consequence to membrane selectivity. This finding defies Maxwell's prediction that the addition of non-permeable spheres will decrease permeability. We aim to investigate the effect of adding nano- and microparticles to other types of polymer, such as rubbery and normal glassy polymers, and the particle size at which composites transition from typical Maxwell behavior to permeability enhancement.

Approach. Polymer films and composites are prepared via solution casting. Each film is characterized with scanning electron microscopy. Transport properties such as the permeability, diffusivity, and solubility coefficients are found using Daynes' lag-time equation. Free volume characteristics are studied through positron annihilation lifetime spectroscopy (PALS). Experimental findings are verified using Accelrys 4.0 Materials Studios modeling program.

SEM micrograph of cross section of PDMS membrane.



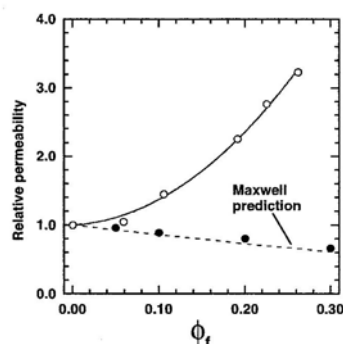
SEM micrograph of cross section of PDMS composite containing amorphous, untreated silica nanoparticles.



Daynes' Lag-Time Equation

$$\frac{P_{\text{downstream}}}{P_{\text{upstream}}} = \left[\frac{A}{Vl} \right] SD \left(t - \frac{l^2}{6D} \right)$$

Addition of nanospheres enhances permeability, which contradicts Maxwell's Theory.



Results. Pure, homogenous poly(dimethyl siloxane) (PDMS), polycarbonate (PC), and poly (ether imide) (PEI) films were successfully prepared. Agglomeration of nanoparticles were present in PDMS composites. Stirring solutions for longer durations reduced agglomerate sizes. Specifications for PDMS modeling were determined.

Future Work. We hope to control and reduce agglomerate sizes by chemically attaching filler particles to polymer chain. Atom transfer radical polymerization (ATRP) provides an effective and relatively simple method to grow polymer chains off the surface of particles, and prepare films with monodisperse particles. Primary silica microparticles will be synthesized via the Stöber process. Experimental and theoretical values of the transport properties and free volume characteristics of pure and composite films will be determined for each polymer classification.

Funding. American Chemical Society Petroleum Research Fund (ACS-PRF).