334h Modeling and Molecular Simulation of Mixed-Matrix Membranes

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Recently mixed-matrix membranes, that nanoporous particles are incorporated into polymer, have shown great interest in separation for gas mixtures. Great improvement of selectivity and permeation could be observed through proper choice of matrix materials and nanoporous particles. We presents the results of molecular dynamics (MD) simulations and modeling of a mixed-matrix membrane composed of polyetherimide and nanosize porous carbon particles. The mixed membrane is composed of 40 monomers and short, open-ended carbon nanotubes representing the porous nano-particles. Dangling bonds of the each end of the nanotubes are saturated with hydrogen atoms. The self-avoiding random walk method of Theodoru and Suter is utilized to generate a three-dimensional periodic simulation cell which contains the polyetherimide polymer and three porous nanoparticles. We use the polymer-consistent force field (PCFF), together with the van der Waals and Coulombic interactions, to model the mixed-matrix membrane. The accessible free volume and radial distribution function of the membrane are calculated and compared with those of pure polyetherimide structure. The self-diffusivity of carbon dioxide and methane are calculated by the NPT-MD simulation at 1 atm. Also computed are the solubility coefficients of the gas molecules. We discuss the effect of porous nano-particles on the self-diffusivities and the solubility coefficients gas molecules. We also investigate fluctuation of pore size of carbon particles.