Molecular Simulation of Gas Permeability of EPE(PEO-PPO-PEO) Triblock Copolymer Membrane

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Molecular simulations were conducted on membrane system that consists of EPE(PEO-PPO-PEO) triblock copolymers with different polyethylene oxide(PEO) wt% for CO_2/N_2 separation. Diffusivity terms were computed using molecular dynamics (MD) simulations and solubility terms using grand canonical Monte Carlo (GCMC) simulations. The simulation results indicate that the permeability and the selectivity of CO_2/N_2 within the EPE system agree well with the experimental data. There is an abrupt increase in the CO2 permeability as PEO content goes to zero due to the structural transformation of the polymer system that enhances diffusion. Finally, the lengths of the polymers were changed to see the effect on the properties of our system.