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Estimation of Mixed-Matrix Membrane Relative Permeability Using Monte Carlo Simulation

Zheng Cao, Haoyu Wu, Boguslaw Kruczek and Jules Thibault
Department of Chemical and Biological Engineering
University of Ottawa, Ottawa, Ontario, Canada K1N 5N6

Extended Abstract

The greater availability of computational power has allowed researchers to investigate the mass transport of a chemical species at various scales of dimension and time from the atomistic to a more macroscopic level. To estimate the relative permeability of mixed-matrix membranes, Monte Carlo (MC) simulations can be used advantageously with respect to the ease of simulation coding and computational time. MC simulation has been used for a large number of applications including studying the migration of species within a membrane. To account for the migration of molecules through a mixed-matrix membrane using MC simulations, a statistically significant and constant number of molecules are allocated on the upstream interface of the membrane (i.e. a constant gas pressure) whereas, for the downstream side of the membrane, molecules exiting the membrane are immediately removed (i.e. a perfect vacuum).

Because the polymeric membrane with embedded nanofillers of a mixed-matrix membrane have different diffusivity and solubility coefficients, the displacement rate and the molecule density in each medium have to be considered to adequately represent the permeation of molecules. The MC simulation is performed in a dynamic mode with where the upstream interface molecules are allowed to freely migrate according to Brownian movement. After a certain number of iterations, the molecule concentration across the membrane and the total population inside the membrane become relatively constant. Under this steady state, the number of molecules entering the upstream interface becomes equal to the number of molecules leaving at the downstream interface.

Results show that the relative permeability, calculated as the ratio of the steady state molecule flux of the mixed-matrix membrane and the steady-state flux of the neat polymeric membrane, is accurate and corresponds to the value obtained by solving the three-dimensional diffusion equation via the finite difference method (FDM). In most cases, the computation time to obtain the same solution with MC simulations is significantly less than with the FDM.