Molecular Simulation of Pressure-Driven Flow of Hydrocarbon Mixtures through Zeolite Membranes

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Abstract:

Selective adsorption in zeolite packed beds is now used in a wide variety of industrial processes to achieve energy-efficient separation of different chemical components. More recently, zeolites have been used in membrane systems. Separation is achieved by selective permeation of a gas mixture under the action of a pressure gradient. Pressure-driven transport of molecules across conventional polymer membranes is usually well-described by the solution-diffusion theory. Molecules dissolve from the feed gas into the membrane on one side, undergo Fickian diffusion through the membrane, and are stripped out by a carrier gas on the far side. The permeation rate of each component depends on only two parameters, the Henry's constant and the Fickian diffusion coefficient. Both of these parameters can be predicted using conventional molecular simulation techniques.

In the case of zeolite membranes at high loadings, the solution-diffusion model is likely to be inadequate. Firstly, we expect to see strong interactions between diffusing molecules as they move through the interior of the zeolite particles. Secondly, the formation of an adsorbed layer at the gas-zeolite interface introduces a non-Fickian transport resistance. Finally, competitive adsorption at the interface can result in significant deviations from Henry's Law.

We are using the dual-control volume grand canonical molecular dynamics method (DCV-GCMD) to simulate pressure-driven permeation across oriented silicalite membranes. Results will be presented for gas feed mixtures containing varying amounts of n-butane, isobutane and neopentane.