

## Separation of Gas Mixtures Using a Range of Zeolite Membranes: A Molecular Dynamics Study

W. Jia and S. Murad<sup>C,S</sup>

*Chemical Engineering Department, University of Illinois at Chicago, Chicago, IL, U.S.A.  
murad@uic.edu*

Gas separation efficiencies of three zeolite membranes (Faujasite, MFI, and Chabazite) have been examined using the method of molecular dynamics. Our investigation has allowed us to study the effects of pore size and structure, state conditions, and compositions on the permeation of two binary gas mixtures,  $O_2/N_2$  and  $CO_2/N_2$ . We have found that for mixture components with similar sizes and adsorption characteristics, such as  $O_2/N_2$ , small-pore zeolites are not suited for separations, and this result is explicable at the molecular level. For mixture components with differing adsorption behavior, such as  $CO_2/N_2$ , separation is mainly governed by adsorption, and small-pore zeolites separate such gases quite efficiently. When selective adsorption takes place, we have found that, for species with low adsorption, the permeation rate is low, even if the diffusion rate is quite high. Our results further indicate that loading (adsorption) dominates the separation of gas mixtures in small pore zeolites, such as MFI and Chabazite. For larger-pore zeolites such as Faujasite, diffusion rates do have some effect on gas mixture separation, although adsorption continues to be important. Finally, our simulations using existing intermolecular potential models have replicated all known experimental results for these systems. This shows that molecular simulations could serve as a useful screening tool to determine the suitability of a membrane for potential separation applications.