192g The Role of Diffusion in Separation of Gas Mixtures Using a Range of Zeolite Membranes: a Molecular Dynamics Study

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The role of diffusion in the 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, O2/N2 and CO2/N2. We have found that for mixture components with similar sizes, such as O2/N2, small-pore zeolites are not suited for separations, and this result is explicable at the molecular level when examining their diffusion rates. For mixture components with differing adsorption behavior, such as CO2/N2, separation is mainly governed by adsorption and small-pore zeolites separate such gases quite efficiently.The diffusion rate in such systems does not play as important a role, since molecules cannot cross each other inside the pore. 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 a significant effect on gas mixture separation, although adsorption continues to be important as well. 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.