Multiscale simulation starting at the molecular level for CO_2/CH_4 separation

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The separation of CO_2/CH_4 is industrially important especially for natural gas processing. In natural gas separation, a CH4-rich residue stream containing less than 2-3% CO_2 is obtained. Carbon molecular sieve (CMS) membranes show excellent separation performance and stability at high temperature and pressure for CO_2/CH_4 separation.

Transport of a confined fluid in CMS is characterized by the coupling of adsorption and diffusion. Quantitative prediction of hindered diffusion is important in guiding experiments and improving engineering designs. Molecular modeling starting at the atomic scale is an efficient tool for quantitatively and qualitatively understanding structure-property relations, and elucidating the mechanisms of microscopic phenomena. In this study, the permeability of CO_2 and CH_4 in a carbon slit pore is predicted within nominal operating temperature and pressure ranges, using grand canonical Monte Carlo (GCMC) and equilibrium molecular dynamics (EMD) simulations.