GCMC and EMD simulation in carbon slit pores for methane

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Using one-site spherical CH4 molecular model, adsorption isotherms obtained from grand canonical Monte Carlo (GCMC) simulation and diffusivities from equilibrium molecular dynamics (EMD) are predicted to calculate permeability in carbon slit pore with the width from 0.65nm to 0.75nm. In the range of temperature from 298K to 318K and pressure from 0.01bar to 80bar, the permeability within the pore width exceeds by 3 orders of magnitude that of reported macroscopic measurements. It is postulated that the pore mouth resistance causes this discrepancy between the slit pore and the real membrane system. The simulation results give an upper bound of the permeability for an ideal carbon membrane.