408c Air Separation by Single Wall Carbon Nanotubes: Thermodynamics and Kinetics

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Separation of a nitrogen-oxygen mixture (air) by single wall carbon nanotubes has been studied using Grand Canonical Monte Carlo and Molecular Dynamics simulations. It is demonstrated that depending on these operating parameters, the extent of adsorptive and kinetic selectivity can vary significantly. Detailed calculations are presented for the adsorption isotherms, self- and transport diffusivities and isosteric heats of pure nitrogen, oxygen and their mixture in a carbon nanotube of 12.53 Å diameter at two temperatures. In mixture adsorption, the energetically favored nitrogen is preferentially adsorbed at low loadings. However, at high loadings oxygen replaces nitrogen due to the dominant entropic effects, and therefore a high adsorptive selectivity towards oxygen is observed close to the saturation loading. The effect of the entropic change on mixture adsorption is evident from the calculated isosteric heats of adsorption. Simulation results were then combined with a continuum description of mass transport to determine the kinetic separation performance of a nanotube membrane. The concentration profiles, diffusivity profiles and membrane fluxes were calculated, and it was demonstrated that by carefully tuning the upstream and downstream pressures, a good kinetic selectivity could be achieved for air separation using single wall carbon nanotubes.