

192e Transport of CO₂ and N₂ through Single-Walled Carbon Nanotube Membranes

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Recent theoretical studies and experimental studies have given indications that carbon nanotubes might be a membrane material with attractive properties quite different to polymeric membranes. We have used atomically detailed simulations to examine the adsorption and transport diffusion of CO₂ and N₂ in single walled carbon nanotubes at room temperature as a function of nanotube diameter. Linear and spherical models for CO₂ are compared, showing that representing this species as spherical has only a slight impact in the computed diffusion coefficients. Our results support previous predictions that transport diffusivities of molecules inside carbon nanotubes are extremely rapid when compared with other porous materials. By examining carbon nanotubes as large as the (40,40) nanotube, we are able to compare the transport rates predicted by our calculations with recent experimental measurements. The predicted transport rates are in reasonable agreement with experimental observations.