

Monte Carlo calculations for the vapor-liquid equilibria of mixtures containing *n*-alkanes, carbon dioxide and dinitrogen

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Abstract

New force fields for carbon dioxide and dinitrogen are introduced that quantitatively reproduce the vapor-liquid equilibria (VLE) of the neat systems and their mixtures with alkanes. In addition to the usual VLE calculations for pure CO₂ and N₂, calculations of the binary mixtures with propane were used in the force field development to achieve a good balance between dispersive and electrostatic (quadrupole-quadrupole) interactions. The transferability of the force fields were then assessed from calculations of the VLE for the binary mixtures with *n*-hexane, the binary mixture of CO₂/N₂, and the ternary mixture of CO₂/N₂/propane. The VLE calculations were carried out using configurational-bias Monte Carlo simulations in either the grand canonical ensemble with histogram reweighting or in the Gibbs ensemble.

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