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Confined phase behavior of a CH4-CO2 binary system: molecular simulations, equation of state, and lattice Boltzmann method

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Phase behavior of confined fluids may deviate significantly from that of the bulk fluid due to the fluid-walls interactions being a significant portion of all intermolecular interactions under confinement. There are recent advancements in understanding confined phase behavior of pure species, confined phase behavior of mixtures remains an understudied topic. In this work, we examine the confined phase behavior of a CH4-CO2 binary system by combining Monte Carlo (MC) simulations, equation of state (EOS), and the lattice Boltzmann method (LBM). First, the effects of confinement on density and phase distribution in nano-sized pores are established using Gibbs Ensemble Monte Carlo (GEMC) calculations, which produces precise results of liquid and vapor confined pressures and accounts for the modification of the phase change location. By comparing the Pxy diagrams of bulk and confined mixtures at a fixed temperature, it is observed that the Pxy diagrams shrink with reductions in pore size. Based on this observation, we extend a modified Peng-Robinson (PR) EOS that was originally developed for pure species to mixtures via a van der Waals-type mixing rule and by incorporating shifts in the critical point of CH4-CO2 mixtures. The resulting phase envelopes are in good agreement with the MC data. Finally, we incorporate this EOS in a multi-component LBM that uses a pseudopotential model to represent intermolecular forces. This work utilizes multiscale simulation techniques to shed light on the confined phase behavior of CH4-CO2 binary systems and to bridge the behavior of multi-component systems across scales.

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Participation

Online

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