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Porosity effects on phase diagram of gas condensate mixture

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A phase diagram of methane+n-butane mixture is investigated by the means of molecular dynamics (MD) simulations. The system exhibits retrograde condensation behavior above 191 K in some range of methane molar fractions. A vapor-liquid equilibrium curve for mixtures is calculated with TraPPE-UA united-atom forcefield [1], TraPPE-EH [2] and OPLS-AA [3,4] all-atom forcefields. The forcefields show good agreement with experimental vaporization curves of pure hydrocarbons. They also reproduce well the composition of liquid phase in binary mixtures as a function of pressure at isotherms, while some discrepancies from experimental data are observed in the saturated vapor compositions. The TraPPE forcefields show better agreement with experimental vapor-liquid equilibrium data than OPLS. The TraPPE-EH accuracy is comparable to that of cubic equations of state.

The effects of nanoscale porosity on mixture phase diagram are qualitatively studied. The saturation curves in slit pores with Lennard-Jones walls are calculated. We considered two sets of wall-molecule interaction parameters and two pore widths. It is shown that nanopores may shift the coexistence curve. At certain wall-molecule interaction parameters, a significant widening of the pressure range of the retrograde condensation is found. This effect may hinder gas extraction from the rocks with a large fraction of nanopores.

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