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Modeling Natural Gas-Carbon Dioxide System for Solid-Liquid-Vapor Phase Behavior

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Abstract

With the shale gas boom, natural gas has become one of the main energy sources in the United States. But in the cryogenic processes of this natural gas, the formation of solid carbon dioxide remains a concern because it can cause the blockage of equipment. Accurately modeling the rich phase behavior of carbon dioxide in methane is helpful for optimizing the industrial processes, especially where experimental data are lacking at the operation conditions. In this work, the Perturbed Chain-SAFT (PC-SAFT) equation of state is applied to model the phase behavior of hydrocarbon (i.e., methane, ethane, butane) + carbon dioxide systems over a wide range of temperatures and pressures. It is observed that the PC-SAFT equation of state can accurately predict the vapor-liquid equilibria (VLE), solid-vapor equilibria (SVE), and solid-liquid equilibria (SLE) of hydrocarbon + carbon dioxide systems using a single set of temperature and pressure independent binary interaction parameters. In the end, the effect of addition of ethane and butane on SLE of methane + carbon dioxide is also investigated which has applications in reducing the carbon dioxide solidification conditions.

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