Data Requirements and Modeling for Gas Hydrate-Related Mixtures and a Comparison of Two Association Models

The association theory-based advanced thermodynamic models have gained more and more attention and applications in many industries. The cubic plus association (CPA) and the simplified perturbed chain statistical associating fluid theory (sPC-SAFT) equations of state (EOS) are two of the most widely used association models in the chemical and petroleum industries. The CPA model is extensively used in flow assurance, in which the gas hydrate formation is one of the central topics. Experimental data play a vital role in validating models and obtaining model parameters. In this work, we will compare the performance of the CPA and sPC-SAFT EOS for modeling the fluid-phase equilibria of gas hydrate-related systems and will try to explore how the models can help in suggesting experimental measurements. These systems contain water, hydrocarbon (alkane or aromatic), and either methanol or monoethylene glycol. It is well known that the determination of SAFT-type model parameters for associating fluids remains a challenge because there are at least five pure-component parameters for these compounds and there is no property combination found to be enough to ensure the best parameter set. Therefore, in this work two parameter sets have been chosen for the sPC-SAFT EOS for a fair comparison. The comparisons are made for pure fluid properties, vapor liquid-equilibria, and liquid liquid equilibria of binary and ternary mixtures as well as vapor liquid liquid equilibria of quaternary mixtures. The results show, from an overall point of view, that these two models have equally good performance, and the two parameter sets with the sPC-SAFT EOS are also comparable, especially for the vapor liquid equilibria systems. Moreover, the modeling results suggest that some data are less reliable than others, which indicates the need for more measurements to further validate the models, especially for multicomponent systems.

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