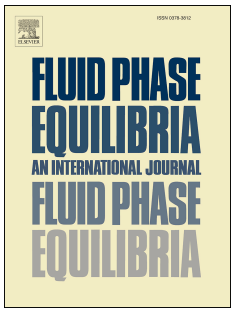

A review on hydrate composition and capability of thermodynamic modeling to predict hydrate pressure and composition

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A review on hydrate composition and capability of thermodynamic modeling to predict hydrate pressure and composition

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Abstract

Gas hydrates are widely considered to be a crucial topic in oil and gas industries and attracting significant research due to potential applications such as gas storage, separation as well as water desalination. While the guest composition of hydrate phase is vital, due to the experimental difficulties in measuring hydrate composition, very little applicable information is available in the literature. Paradoxically, this is true, in spite of that; completing an experimental database on hydrate composition could have a significant impact on the processes design and modeling. Moreover, this should provide fundamental knowledge of kinetic effects as well as clarifying thermodynamic equilibrium. Hence, this paper was planned with the intent to fill in the gaps, classify and offer an overview of experimentally derived data on hydrate composition for literature. In addition, a thermodynamic model based on the van der Waals and Platteeuw approach and Kihara potential was utilized to simulate the hydrate composition along with equilibrium pressure.

Previous experimental data shows that guest distribution in hydrate phase depends noticeably on the guest composition in vapor phase. In addition, composition of larger molecules, such as propane or butane, in the hydrate phase, is notably higher than in vapor phase. Our simulation results demonstrates that the hydrate composition data from direct measurement (microscopic tools) have been well evaluated by the thermodynamic model. Nevertheless, when structural transition can occur in a system, the thermodynamic model is no longer accurate. In the case of indirect measurements, the thermodynamic model usually predicts well the hydrate composition. Nonetheless, its capability does vary with differing hydrate composition and equilibrium pressure, to the extent that in some cases, it completely fails to predict hydrate composition. This could be due to kinetic effects on the enclathration of guest molecules during the crystallization, errors in experimental techniques to measure the hydrate composition or the model parameters like Kihara potential are not properly applied. Finally, these observations show that more reliable experimental database is needed to study the evolution of guest distribution in hydrate phase and some enhancements are required for the standard thermodynamic model.