A New Model for Mixed Hydrates Consistent with Multiparameter Equations of State

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In this work, the model for pure hydrates (water + one hydrate forming substance) that was developed by our group [1–3] has been extended to systems with more than one hydrate forming substance in the mixture (mixed hydrates). The refined model can represent high pressure three-phase equilibrium data for which guest molecules are known to double occupy cavities. It is intended for modeling of mixed hydrates in carbon capture and storage (CCS)-relevant mixtures. For the newly developed mixed hydrate model, a simple mixing rule for the volume is used, which does not contain any adjustable parameters. The new model is consistent with accurate multiparameter equations of state for fluid phases of the corresponding mixtures. Comparisons of the new model to experimental data for mixed hydrates are presented for several multicomponent mixtures containing substances that are relevant for the intended application. The influence of double occupied cavities on calculated phase equilibria as well as the improvements for calculated three-phase hydrate formation temperatures at pressures, where double cage occupancy occurs, are shown for argon, nitrogen, oxygen, and air. It has been observed that pure guest components forming a certain structure may form another hydrate modification when present in a mixture [4,5]. With the refined algorithms for the stability analysis, it will be shown which hydrate structure is found to be more stable at the given conditions. The results are compared to experimental results.

References:

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