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Thermodynamic Model for Prediction of Phase Equilibria of Gas Hydrates in the Presence of Water-Insoluble Organic Compounds

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Abstract

A thermodynamic model for predicting pressure – temperature phase diagrams of structure II and structure H clathrate hydrates of methane, carbon dioxide, or hydrogen sulfide in the presense of "water-insoluble" organic componds is presented. The model is based on equality of water fugacity in the aqueous and hydrate phases. The solid solution theory of van der Waals – Platteeuw (vdW-P) is used for calculating the fugacity of water in the hydrate phase. The Peng-Robinson (PR) equation of state (EoS) is employed to calculate the fugacity of the compounds in gas phase. It is assumed that the gas phase is water and promoter free and the organic compounds do not have considerable effects on water activity in liquid phase. The results of this model are finally compared to existing experimental data from the literature. Acceptable agreement is found between the model predictions and the investigated experimental data.

Keywords: Gas hydrate, Thermodynamic model, Van der Waals – Platteeuw theory, Phase equilibria, Water-Insoluble Organic Compounds

Research Highlights

- A thermodynamic model has been developed for for predicting P–T phase diagrams of binary clathrate hydrates.
- The binary clathrate hydrates include methane, CO2 or H2S + various heavy hydrate formers.
- The model is based on the solid solution theory of van der Waals – Platteeuw combined with the PR-EoS.