Modeling Gas Hydrates Using the PRSV EoS and the vdW-P Model

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Gas hydrates are ice-like crystalline solids in which water molecules form a three-dimensional structure that is stabilized by the encapsulation of small gas molecule like methane, ethane and carbon dioxide. The motivation of this work is to build a calculational model to predict the vapor-liquid-hydrate three-phase equilibrium condition with a better degree of predictability.

In this study, the van der Waals and Platteeuw (vdW-P) model [1] is applied to describe the hydrate phase and the Peng-Robinson-Stryjek-Vera (PRSV) equation of state (EoS) is chosen [2] to describe the vapor and liquid phases. In the vdW-P model, the Langmuir adsorption behavior is assumed to model the adsorption of gas molecules in the hydrate cages, and the Langmuir constant is defined as a function of the spherically symmetric cell potential function. In this study, the Langmuir constant is described by a two-parameter temperature-dependent function. It is found that the vapor-liquid-hydrate three-phase equilibria can be well described by this simple model.

[1] J.H. van der Waals, J.C. Platteeuw, Advances in Chemical Physics 2 (1959) 1-57.
[2] R. Stryjek, J.H. Vera, Canadian Journal of Chemical Engineering 64 (1986) 323-333.