

Determination of the Global Phase Behavior of THF + CH₄, +CO₂, and + H₂O Binary Mixtures using the SAFT-VR Approach

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The optimization of processes involved in enhanced natural gas recovery from sources as gas hydrates have gained media attention. Tetrahydrofuran (THF)-hydrates are interesting because the presence of THF decreases the hydrate stability pressure by approximately two orders of magnitude [1]. Thus, a preliminary detailed knowledge of behavior of binary mixtures containing water (H₂O), carbon dioxide (CO₂), methane (CH₄) and tetrahydrofuran (THF) plays a central role in this context. In this work, the molecular based Variable Range Statistical Associating Fluid Theory (SAFT-VR EoS [2,3]) has been used to estimate the global phase equilibria diagram of the binary mixtures THF+CH₄, THF+CO₂ and THF+H₂O over the whole composition, pressure and temperature ranges. To describe this complex multicomponent mixtures CO₂ molecule [4] is modelled as two spherical segments tangentially bonded, CH₄ [5] as a spherical segment, and H₂O [6] as a spherical segment with four associating sites to represent hydrogen bonding. For the case of THF, different models have been tested to model the correct interactions with the named substances. For example, a simple spherical segment model of tetrahydrofuran [7] has been used to represent his interaction with CH₄ and CO₂. Nevertheless, a THF molecule modelled as a spherical segment with two associating sites has been used to represent correctly the complex interaction THF-H₂O. The THF+ CO₂, THF+CH₄ and THF+H₂O binary mixtures exhibit type I, type III and type VI behavior respectively, according to the classification of Scott and van Konynenburg. Finally, the SAFT-VR phase binary diagrams predictions three-phase were compared to experimental results.

References

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