

Accepted Manuscript

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PII: S0263-8762(17)30618-4
DOI: <https://doi.org/10.1016/j.cherd.2017.11.015>
Reference: CHERD 2894

To appear in:

Received date: 27-4-2017
Revised date: 1-10-2017
Accepted date: 6-11-2017

Please cite this article as: Beheshtimaal, Arghavan, Haghtalab, Ali, Thermodynamic modeling of hydrate formation conditions using different activity coefficient models in the presence of tetrahydrofuran (THF). Chemical Engineering Research and Design <https://doi.org/10.1016/j.cherd.2017.11.015>

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Thermodynamic modeling of hydrate formation conditions using different activity coefficient models in the presence of tetrahydrofuran (THF) *Arghavan*

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Highlights

- A thermodynamic modeling is developed to correlate the hydrate formation conditions of single and binary gases
- The models of NRTL, NRTL-NRF, UNIQUAC and UNIQUAC-NRF were applied for nonideality of the aqueous phase
- The hydrate formation conditions for the CH₄-THF, CO₂-THF and CH₄-C₂H₆-THF hydrate systems were also correlated
- The results showed that NRTL-NRF models give better results for single gas systems and UNIQUAC for the gas-THF systems.
- The UNIFAC group contribution model is also used for both single gas and gas-THF hydrate systems

Abstract

The clathrate hydrate is a major problem in gas transportation lines and on the other hand, can be used as a tool for natural gas storage. Moreover, it could be used for gas separation such as monoxide and dioxide carbon from combustion chambers. In this work, a thermodynamic model is developed to calculate gas hydrate formation conditions of single and binary gases in the absence and presence of the thermodynamic promoter such as tetrahydrofuran (THF). A three-phase solid-liquid-gas equilibrium calculation is carried out so that the van der Waals-Platteeuw model is applied for the hydrate phase, SRK EoS for the gas phase and the different activity coefficient models such as local composition and group contributions models for the aqueous solution. The binary interaction parameters for the

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