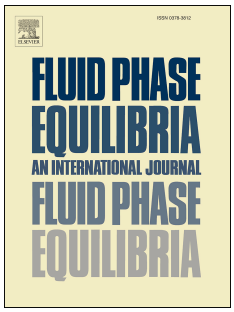

Thermodynamic modeling of methane hydrate formation in the presence of imidazolium-based ionic liquids using two-step hydrate formation theory and CPA EoS

Sadegh Ahmadian, Mohsen Mohammadi, Mohammad Reza Ehsani

PII: S0378-3812(18)30268-1

DOI: 10.1016/j.fluid.2018.07.004

Reference: FLUID 11881

To appear in: *Fluid Phase Equilibria*

Received Date: 30 April 2018

Revised Date: 3 July 2018

Accepted Date: 4 July 2018

Please cite this article as: S. Ahmadian, M. Mohammadi, M.R. Ehsani, Thermodynamic modeling of methane hydrate formation in the presence of imidazolium-based ionic liquids using two-step hydrate formation theory and CPA EoS, *Fluid Phase Equilibria* (2018), doi: 10.1016/j.fluid.2018.07.004.

Thermodynamic modeling of methane hydrate formation in the presence of imidazolium-based ionic liquids using two-step hydrate formation theory and CPA EoS

Sadegh Ahmadian, Mohsen Mohammadi*, Mohammad Reza Ehsani

Department of Chemical Engineering, Isfahan University of Technology, Isfahan 84156-83111, Iran

*E-mail: mohsen_mohammadi@cc.iut.ac.ir

Abstract

In this study, thermodynamic modeling is performed to predict the P-T equilibrium conditions of methane gas hydrate formation in presence of ionic liquids. The imidazolium-based ionic liquids including [EMIM][HSO_4], [EMIM][$EtSO_4$], [BMIM][BF_4], [OH-EMIM][BF_4], [BMIM][Cl] and [BMIM][Br] are modeled through two-step hydrate formation theory of Chen and Guo coupled with CPA EoS for calculating the fugacities of species in liquid and gas phase. The CPA pure component parameters for ionic liquids and also the majority of binary interaction parameters are adjusted using the liquid density and binary VLE data, respectively. The thermodynamic modeling is carried out in the presence of 0.1 weight fractions of all the studied imidazolium based ionic liquids. Moreover, the effect of three various concentrations of [BMIM][BF_4] on the P-T equilibrium diagram of methane hydrate are predicted at 0.1, 0.15 and 0.20 weight fractions of this ionic liquid. The results indicate that the CPA EoS can satisfactorily model the phase behavior of aqueous solutions of imidazolium based ionic liquids considering 2B scheme for the association term. In addition, the results indicate good predictions of the proposed model for methane hydrate equilibrium conditions in the presence of imidazolium-based studied ionic liquids including concentration changes such that the absolute average deviations of methane hydrate formation pressures is obtained below 4.2%.

Keywords: Gas hydrate, Phase equilibria, Imidazolium based ionic liquids, two-step hydrate formation theory, CPA EoS