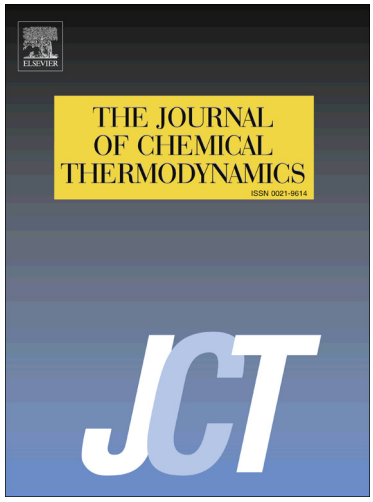

Accurate thermodynamic description of vapor-liquid and solid-liquid equilibria of THF, water and gas hydrates with a unique set of parameters

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Accurate thermodynamic description of vapor-liquid and solid-liquid equilibria of THF, water and gas hydrates with a unique set of parameters.

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Abstract

In the context of gas hydrates technology for gas storage and separation processes, tetrahydrofuran (THF) has a recognized performance as a thermodynamic promoter. Literature presents a large amount of phase equilibrium experimental data for the THF hydrates systems, however, a consistent thermodynamic modeling capable of describing vapor-liquid, liquid-hydrate and liquid-ice equilibria of THF and water is still needed.

With the goal of obtaining this needed modeling, we propose a strategy for the estimation of a unique set of parameters for suitable thermodynamic models for THF and water mixtures in the conditions of vapor, liquid and hydrate. To perform phase equilibrium calculations, we selected the NRTL G^E model, the Peng-Robinson equation of state and the van der Waals and Platteeuw hydrate model with the Kihara potential to correlate independent properties. We regressed parameters for the NRTL and Kihara models in two sequential steps using experimental data at conditions with pressure from 40 kPa to 101.33 kPa and temperature from 272.00 K to 343.15 K. The first steps determines optimal parameters for NRTL with, simultaneously, vapor-liquid equilibria and infinite dilution activity coefficient data. The second determines optimal Kihara paramters with liquid-hydrate equilibria data using a data reconciliation methodology. We verified the potential of the model for extrapolation by accurately describing phase equilibria scenarios involving liquid and vapor mixtures not included in the regression procedure, in addition to scenarios involving conventional ice and hydrates of THF with some industrial gas or natural gas components: H_2, CO_2 or CH_4.

Keywords: hydrates, solid-liquid equilibrium, vapor-liquid equilibrium, tetrahydrofuran, parameter estimation.