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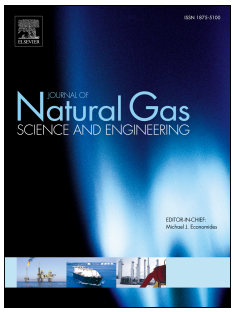

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Mean Activity Coefficient of Electrolytes: A Critical Evaluation of Four Physical Models

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Abstract

Accurate prediction of phase equilibria in the presence of electrolytes is important for many applications. For hydrate phase equilibria in the presence of salts, the fluid phase equation of state needs to be coupled with a reliable electrolyte model. In this work, various electrolyte models: Debye-Hückel, truncated Debye-Hückel, Pitzer theory and Bromley activity models have been critically evaluated for predicting the mean activity coefficient for various aqueous salt solutions. The Debye-Hückel and truncated Debye-Hückel models give accurate predictions at lower salt concentrations, but a large deviation was observed at molal concentrations higher than about 1 mol/kg. The Bromley activity model and Pitzer theory were found to be good alternatives to the Debye-Hückel models and its modifications. For 1:1 electrolytes, the Pitzer theory and Bromley activity models give accurate predictions up to the saturation limit of salt solutions. Conversely, mean activity coefficient calculations for 1:2 electrolytes ($CaCl_2$, $MgCl_2$ and $BaCl_2$) using the Pitzer theory, Bromley activity model, or Debye-Hückel model and its modification were not able to capture the electrolyte contribution of these salts.

***Keywords*:** Electrolytes, Mean activity coefficient, Debye-Hückel model, Pitzer theory, Bromley activity model

1. Introduction

Accurate prediction of phase equilibria in the presence of electrolytes is important for many applications such as hydrometallurgy [1], desalination [2], ion-exchange processes [3], Li-ion batteries [4], and clathrate hydrates of natural gases [5]. Deepwater explorations and extraction

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