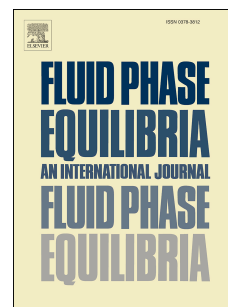


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Modeling the solubility of CO₂ in aqueous methyl diethanolamine solutions with an electrolyte model based on COSMO-RS

Thomas Gerlach^{a,*}, Thomas Ingram^b, Georg Sieder^b, Irina Smirnova^a

* corresponding author (thomas.gerlach@tuhh.de)

^a Hamburg University of Technology, Institute of Thermal Separation Processes, Eißendorfer Straße 38, D-21073 Hamburg, Germany

^b BASF SE, GCP/TD – L540, 67056 Ludwigshafen, Germany

keywords: COSMO-RS, electrolyte systems, carbon dioxide, MDEA, partial molar enthalpies

Abstract

A new COSMO-RS based electrolyte model (COSMO-RS-ES) was applied to the prediction of the solubility of CO₂ in aqueous MDEA solutions. For this purpose, the model was combined with the Soave-Redlich-Kwong equation of state to describe the gas phase non-ideality. First, it was shown that the model can successfully describe the phase equilibria in the CO₂ + water, as well as in alkanolamine + water systems. Using a region specific interaction parameter for the amine, the accuracy of the model for the prediction of the phase equilibrium in alkanolamine + water systems was further improved. Additionally, a detailed investigation of different amine + water systems based on the calculation of the partial molar enthalpies and entropies provided valuable insights on the properties of the systems. The description of the ternary CO₂ + MDEA + H₂O system was successful after a readjustment of selected interaction energy equations of the model using few parameters. The model was then applied to the prediction of the species distribution as well as the prediction of the partial pressure of CO₂ at low gas loading.

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