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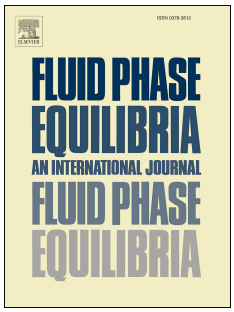

Modelling the solubility of CO_2 in aqueous methyl diethanolamine solutions with an electrolyte model based on COSMO-RS

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Modeling the solubility of CO_2 in aqueous methyl diethanolamine solutions with an electrolyte model based on COSMO-RS

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Abstract

A new COSMO-RS based electrolyte model (COSMO-RS-ES) was applied to the prediction of the solubility of CO_2 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 CO_2 + 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 CO_2 + MDEA + H_2O 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 CO_2 at low gas loading.