Simultaneous Description of Activity Coefficients and Solubility with eCPA - DTU Orbit (12/12/2018)

Simultaneous Description of Activity Coefficients and Solubility with eCPA

In the many developments of electrolyte equations of state presented over the past decades, several different properties have been in focus. A property that has not been widely used as a fitting property is salt solubility. This work presents a new parametrization of the eCPA equation of state with salt specific parameters. The focus is on accurate description of the salt solubility, and low deviation correlations are obtained for all salts investigated. The inclusion of the solubility data in the parametrization has, compared to parameters only parametrized to osmotic coefficients and activity coefficients, not significantly affected the deviations of the osmotic coefficients and activity coefficients. The average deviations of the activity coefficient does increase slightly and it was found that the increase in deviations was almost entirely due to reduced accuracy at high temperature and high molality. The model is, furthermore, compared to the activity coefficient model, Extended UNIQUAC. It is shown that the eCPA provides more accurate solubility description at higher temperatures than Extended UNIQUAC but also that Extended UNIQUAC is slightly better at describing the activity coefficients. Overall the two models perform similarly.

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