Analysis and modeling of alkali halide aqueous solutions - DTU Orbit (08/11/2017)

Analysis and modeling of alkali halide aqueous solutions

A new model is proposed for correlation and prediction of thermodynamic properties of electrolyte solutions. In the proposed model, terms of a second virial coefficient-type and of a KT-UNIFAC model are used to account for a contribution of binary interactions between ion and ion, and water and ion, respectively, with a Debye-Hückel term for electrostatic interactions. In a second approach of the model, additional parameters for interactions of ion pairs in the KT-UNIFAC are introduced as a correction to get better agreement with data. Structural parameters of ions used in the framework of UNIFAC or UNIQUAC are newly estimated using ionic radii for physically correct representation of the combinatorial part. Including temperature-dependent coefficients in the interaction parameters, significant improvements in accuracy are achieved for a wide range of temperatures. This work is focused on calculations for various electrolyte properties of alkali halide aqueous solutions such as mean ionic activity coefficients, osmotic coefficients, and salt solubilities. The model covers highly nonideal electrolyte systems such as lithium chloride, lithium bromide and lithium iodide, that is, systems that are very soluble in water, for example, up to more than 30 mol kg-1. Phase behaviors for the systems are analyzed at concentrations of salt up to the solubility in water at temperatures between 273 and 373 K by comparing calculated results with available experimental data and available models.

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