Refinement of COSMO-RS for the calculation of phase equilibria in electrolyte solutions of mixed solvents

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For various separation processes electrolyte systems are of high importance. Due to their different nature ionic species, in comparison to non-electrolytes, pose challenges towards the development of efficient separation techniques.

The knowledge on the thermodynamic data of systems including the influence of electrolytes in different solvent mixtures and the capability to model these systems is crucial to speed up the development of such separation processes.

An effective model to predict phase equilibria in systems without prior knowledge of the properties of different systems is COSMO-RS. It relies on quantum chemistry, statistical thermodynamics and on a general description of the interactions between the molecules. However, refinements of the model are necessary to describe electrolyte systems.

The aim of this work is to modify the model to improve the description of phase equilibria in electrolyte systems. Several types of systems are taken into account with an emphasis on solid-liquid-equilibria of salts in mixtures of aqueous and organic solvents.

Figure 1: Calculation of solid-liquid-equilibria on the basis a version of COSMO-RS adjusted to electrolytes