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Electrolytes



Poster



THE (WATER + ALCOHOL + ALKALI HALIDE) MIXED-SOLVENT ELECTROLYTE SYSTEMS: DATA STATUS AND CONSISTENCY ANALYSIS USING ELECTROLYTE-NRTL MODEL

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Abstract:

Modelling of the thermodynamic properties of mixed-solvent electrolyte systems is particularly challenging. In terms of theory, the complexity originates from the very different interactions between molecule and molecule, molecule and ion, and ion and ion, and the very different solvation extent of water and organic solvent around the ions. In terms of experiment, datasets were published in different conventions that were not always clearly stated, and are difficult to reconcile. In terms of modelling, the traditional water-based reference-state framework and concentration unit definitions are not practical, as the organic solvent is treated as a solute even for mixtures with very low water concentration (and thus very high co-solvent concentration).

The aim of this work is to analyse data of the thermodynamic properties of mixed-solvent electrolyte systems through an extensive database in terms of internal and external consistency. We will use this analysis to discuss reference state and concentration definitions that are suitable for mixed-solvent electrolyte mixtures over large concentration ranges (both salt and co-solvent), and to present a benchmark database for future equation of state modelling.

The investigated properties include vapour-liquid equilibrium (VLE), liquid-liquid equilibrium (LLE), solid-liquid equilibrium (SLE), and mean ionic activity coefficients (MIAC). Experimental datasets are summarized. Data distributions are shown. The data status is not as extensive as for binary (water + salt) mixtures, but is quite adequate for data consistency analysis among the same family of salts, at least for (water + methanol) and (water + ethanol) co-solvents. The electrolyte-NRTL model is used to convert various properties to the MIAC and water activity coefficient (WAC). In this way, the various properties are reconciled. It is shown that it is possible to use a single e-NRTL parameter to analyze the solvation behaviour of mixed solvents. Doing so, the trend of this parameter is investigated for each ternary mixture.

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