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On the Thermodynamic Properties of Mixed-Solvent Electrolytes Using the SAFT-VR+DE Equation of State

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Abstract

We apply the SAFT-VR+DE equation of state to the study of experimental mixed-solvent electrolyte solutions. In the non-primitive model based SAFT-VR+DE approach (Zhao et al., JCP **2007**, *126*, 244503) the ions are considered fully dissociated within the solvent, which is explicitly treated within the model and the theoretical framework. Typically in the study of electrolyte systems the simpler primitive model is used, which requires knowledge of the experimental dielectric constant. With the non-primitive model the dielectric constant is calculated as part of the theory, which is a particularly attractive feature in the study of mixed-solvent electrolyte systems as data for the experimental dielectric constant of these systems is more scarce. Here for the first time as far as the authors are aware, a non-primitive based equation of state has been used for the study of mixed-solvent electrolytes. The solvents considered (water, methanol and ethanol) are modeled using the SAFT-VR+D approach (Zhao et al., JCP **2007**, *127*, 084514; Zhao et al., JCP **2006**, *125*, 104504) in which the contribution of the dipole to the thermodynamics and structure of the fluid are explicitly accounted for. The theory is found to accurately predict the vapor-liquid equilibrium, as well as dielectric properties of the salt free alcohol-water mixtures both at room and elevated temperatures. Ternary mixtures of salt/water/alcohol are then studied using the SAFT-VR+DE parameters for the salts determined in earlier work (Das et al., AIChE Journal **2015**, *61*, 3053-3072) and a cation-alcohol unlike dispersive energy parameter obtained by fitting to mean ionic activity coefficient data at room temperature and pressure. Thus, with only one adjustable parameter, a predictive SAFT-VR+DE equation to study mixed-solvent electrolyte systems is developed. The SAFT-VR+DE predictions are found to be in good quantitative agreement with mean ionic activity coefficient data for several mixed-solvent electrolyte systems over a wide range of molalities and different solvent ratios. The model is parameterized to allow the molecular level interactions between different cations and the surrounding solvent molecules to be explored.

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