Modeling the Thermodynamic Phase Behavior of Charged fluids using the SAFT-VR+DE EOS

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Understanding the non-ideal thermodynamic behavior of charged systems is essential for the design and development of many important chemical, biological and environmental processes and has resulted in an increasing demand for predictive tools that accurately describe the thermodynamic behavior of such systems. In this regard, molecular-based equations of state, such as the statistical associating fluid theory (SAFT), which are able to describe the thermodynamic behavior of fluids using adjustable physically based parameters, can be considered a powerful tool to describe the thermodynamics of complex systems. In recent work the statistical associating fluid theory for potentials of variable range (SAFT-VR) [1] equation of state, was extended by the authors [2] to explicitly incorporate electrostatic interactions (i.e., ion-ion, ion-dipole and dipole-dipole) using the mean spherical approximation of Blum et al. [3] with the non-primitive model to describe the solvent molecules. In this work, we apply this extension to deal with pure fluids and mixtures of charged fluids, such as electrolytes, mixed solvent electrolytes and ionic liquids.

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