

A Statistical Associating Fluid Theory for Strong Electrolyte Solutions

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The statistical associating fluid theory (SAFT) [1, 2] has proven to be a powerful equation of state for modeling complex fluids and their mixtures. In the present work, we extended a version of the SAFT-VR [3] equation, which models non-conformal fluids with potentials of variable attractive range, to represent the density, vapor pressures, and salting-out of several aqueous strong electrolytes. In the proposed equation, water is modeled as a dipolar square-well sphere with four associating sites to mimic hydrogen-bonding interaction, and the experimental value of the dipole moment is used. Strong electrolytes are considered, and are therefore treated as fully dissociated. The cation and anion are modeled as hard spheres of different size, with values corresponding to the experimental Pauling radii for each ion. The mean spherical approximation (MSA) is used to describe the long-range Coulombic ion-ion, ion-dipole, and dipole-dipole interactions. Within the ion-dipole non-primitive model, the solvent effect is explicitly taken into account and not represented as a dielectric continuum medium, as in the SAFT-VRE equation [4] and other SAFT based equations [5] for electrolyte solutions. Good agreement is obtained between the theoretical calculations and the experimental data for the density and vapor of several aqueous strong electrolytes. Additionally, the approach describes the salting-out effect of aqueous strong electrolytes well, using SAFT-VR parameters for gases obtained in our earlier work [6].

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