An Electrolyte Lattice Fluid Equation of State Applicable to Electrolyte Solutions

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Curent interests in thermodynamic properties are on complex systems including electrolytes. For high-pressure or phase equilibria containing supercritical gases, however, excess Gibbs energy models are not adequate. Properly formulated equation of state approaches should yield thermodynamic properties of concentrated solutions if solvations are accounted for in the model and of high pressure systems.

In the present study, the Helmhotz free energy model is approximated as a sum of physical, association, and long-range contributions. The physical and association contributions were modeled using non-random lattice fluid theory with hydrogen bonding. A MSA model was used to describe the long-rang contributions in electrolyte solutions. For each ions, segment number and interaction energy parameters were used. Besides, hydration energy and number were used to describe the solvation between cations and solvents. The Electrolyte lattice fluid EOS was applied to calculate osmotic coefficients, mean activity coefficients, and densities of electrolyte solutions.