Equations of State for Multi-Component Solutions of Electrolytes Using Ion-Specific Parameters

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Equations of state have been implemented and studied for multi-component electrolyte solutions at different temperatures and pressures. The equations are expressed in terms of the Helmholtz free energy and contain terms accounting for short-range and long-range interactions in electrolyte solutions.

Short range interactions are described by one of the three equations of state: Peng-Robinson, Soave-Redlich-Kwong, or Cubic-Plus-Association (CPA). Long range interactions are described by either the simplified mean spherical approximation (MSA) solution of the Ornstein–Zernicke equation or the simplified Debye-Hückel term. An optional Born term is added to these electrostatic terms.

The resulting electrolyte equations of state were tested by determining the optimal model parameters for the multi-component system consisting of H_2O, Na , H , Ca_2 , Cl^-, OH^-, SO_4^{2-}, CO_3^{2-}, HCO^{3-}, CO_2, and methanol.

In order to describe the thermodynamics of this multi-component system, ion-specific parameters were determined. The parameters in the equations of state were fitted to experimental data consisting of apparent molar volumes, osmotic coefficients, solid-liquid equilibrium data, vapor-liquid equilibrium data, and thermal property data.

The results of the parameter fitting are presented. The ability of the equations of state to reproduce the experimental data is demonstrated. The performance of the equations of state for multi-component systems is compared and analyzed in view of the various short range and long range terms employed.