Modeling Acid-Base Equilibria and Phase Behavior in Mixed-Solvent Electrolyte Systems

P. Wang, J.J. Kosinski, R.D. Springer, and A. Anderko[C,S]
OLI Systems Inc, Morris Plains, NJ, U.S.A.
aanderko@olisystems.com

A previously developed thermodynamic model for electrolyte systems has been applied for the simultaneous computation of acid-base and phase equilibria in systems containing water, salts, and nonaqueous solvents (e.g., hydrogen peroxide, alcohols and glycols). The model combines an excess Gibbs energy model with detailed speciation calculations. The excess Gibbs energy model consists of a long-range interaction contribution represented by the Pitzer-Debye-Hückel expression, a short-range term expressed by the UNIQUAC model, and a newly developed second-virial-coefficient type term for specific ionic interactions. Particular attention has been focused on the self-dissociation behavior of nonaqueous and mixed solvents and its impact on measurable properties such as pH. The model has been extensively verified using pH and spectroscopic measurements as well as solid-liquid, liquid-liquid, and vapor-liquid equilibrium data.