Modeling Phase Equilibria and Solution Chemistry in Multiphase, Multicomponent Electrolyte Systems

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A previously developed comprehensive model for mixed-solvent electrolyte solutions has been applied to systems that exhibit complex phase behavior, including the presence of two liquid phases with partially ionized components and multiple competing solid phases. The computational framework combines an excess Gibbs energy model, a model for standard-state properties of solution species, and an algorithm for solving phase and chemical equilibria in multicomponent, multiphase systems. The model has been applied to, among others, systems that are involved in hydrogen production through thermochemical cycles (e.g., the iodine – sulfur cycle), ionic liquids, and systems containing natural brine components in the presence of alcohols and glycols. In particular, emphasis has been put on developing a methodology for determining meaningful model parameters. Speciation models have been developed to represent simultaneously thermodynamic and transport properties of concentrated solutions.