

Modeling Speciation and Phase Equilibria of Aqueous Boric Acid and Metal Borates from Ambient to Hydrothermal Conditions

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Detailed understanding of the thermodynamic behavior of boric acid and metal borates in aqueous environments is important for modeling nuclear power reactor chemistry, geothermal fluid chemistry, and processes for the recovery of critical materials (in particular, lithium) from brines. To address these needs, a comprehensive model has been developed for simultaneous phase equilibrium and speciation calculations in wide temperature, pressure, and concentration ranges. The new model utilizes detailed speciation results from recent electrical conductivity measurements in dilute boric acid and alkali metal borate solutions and quantitative Raman spectroscopic studies at moderate concentrations. The model has been constructed based on the Mixed-Solvent Electrolyte (MSE) framework, which has been parameterized for systems containing boric acid and the borates of lithium, sodium, potassium, calcium and magnesium by combining the new speciation data with vapor-liquid equilibrium and solid solubility data. The MSE model incorporates a treatment of standard-state properties of simple and complex aqueous species and an excess Gibbs energy model that is valid up to solid-liquid saturation or the fused electrolyte limit. This approach ensures the correct prediction of the formation of experimentally identified polyborate species while reproducing extensive experimental solubility and vapor-liquid equilibrium data. The model has been validated for temperatures up to 623 K at widely varying metal / boron ratios. In particular, the model aligns with the new experimental speciation results to provide reliable predictions under the conditions of pressurized water reactors (PWRs) for nuclear power generation.