Rare-Earth Elements in Aqueous Sulfate Systems: Thermodynamic Modeling of Binary and Multicomponent Systems in Wide Concentration Ranges

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A comprehensive model has been developed for calculating thermodynamic properties and phase equilibria in binary and multicomponent aqueous systems containing rare earth element sulfates. The model encompasses yttrium and all lanthanides except promethium. The model has been parameterized and verified using a database that includes solid-liquid equilibria, osmotic coefficients, enthalpies of dilution and heat capacities of solutions. The computational framework is based on the previously developed Mixed-Solvent Electrolyte (MSE) model. Phase equilibria have been accurately reproduced for binary rare earth sulfate – water systems and for ternary mixtures that additionally include sulfuric acid and/or sodium sulfate. Solid-liquid phase diagrams have been generated to provide a convenient summary of the solubility of stable and metastable hydrated solid phases. Analysis of the stability of solid hydrates reveals systematic trends within the rare earth series. Rare-earth elements can be recovered from solution in the form of sparingly soluble double sodium - rare earth – sulfate salts. It has been shown that the solubility of the double salts reaches a minimum for praseodymium and appreciably increases for heavier rare earth elements, thus making the separation via precipitation most effective for praseodymium and neodymium and less effective for heavier elements.