## PHREEQ-N-AMDTreat+REYs Water-Quality Modeling Tools to Evaluate Acid Mine Drainage Treatment Strategies for Recovery of Rare-Earth Elements

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## **Abstract**

The PHREEQ-N-AMDTreat+REYs water-quality modeling tools have the fundamental capability to simulate aqueous chemical reactions and predict the formation of metal-rich solids during the treatment of acid mine drainage (AMD). These new user-friendly, publicly available tools were expanded from the PHREEQ-N-AMDTreat tools to include the precipitation of rareearth elements plus yttrium (REYs) and the adsorption of REYs onto hydrous Fe, Al, and Mn oxides. The tool set consists of a caustic titration model that indicates equilibrium surface and aqueous speciation of REYs as functions of pH and caustic agent, and a kinetics+adsorption model that simulates progressive changes in pH, major ions, and REYs in water and solids during sequential steps through passive and/or active treatment. Each model has a user interface (UI) that facilitates the input of water-quality data and adjustment to geochemical or treatment system variables; for example, retention time and aeration rate are adjustable parameters in the kinetics model. On-screen graphs display results of changes in metals and associated solute concentrations as functions of pH or retention time; details are summarized in output tables.

A goal of such modeling is to identify strategies that could produce a concentrated REYs extract from AMD or mine waste leachate. For example, if REYs could be concentrated after first removing substantial Fe and Al, the final REYs-bearing phase(s) could be more efficiently processed for REYs recovery and, therefore, may represent a more valuable commodity. Preliminary modeling supports the hypothesis that Fe and Al can be removed at pH < 5.5 using conventional sequential oxidation and neutralization treatment processes without removing REYs, and that further increasing pH can promote the adsorption of REYs by hydrous Mn oxides. Alternatively, chemicals such as oxalate or phosphate may be added to precipitate REYs compounds following initial steps to decrease Fe and Al concentrations. The aqueous geochemical model framework is comprehensive and permits evaluation of effects from interactive chemical and physical variables. Field studies that demonstrate REYs attenuation from AMD and corresponding solid-phase formation during specific treatment steps plus laboratory studies of aqueous/solid interactions are helpful to corroborate, refine, and constrain modeling parameters.

Keywords: resource recovery, adsorption, precipitation, equilibrium, kinetics