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The MINES thermodynamic database: geochemical modeling of hydrothermal ore-forming processes and stability of critical minerals

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Geochemical modeling of fluid-rock interaction yields important insights in the stability of minerals, their solid solutions, and the speciation of aqueous complexes and gases. Accurately modeling the geochemistry and mineralogy observed in ore deposits and other fluid-rock systems requires robust thermodynamic datasets valid in non-ideal system and in a broad range of pressure, temperature, and fluid compositions. Here we present an updated version of the MINES thermodynamic database (https://geoinfo.nmt.edu/mines-tdb/) that has been available open access for more than a decade. The database is implemented in the geochemical modeling program GEMS (https://gemshub.github.io/site/) and a new version will be available for easy distribution in other formats including .csv files and the PHREEQC database for integration with other geochemical modeling programs. MINES contains a wide array of rock forming minerals, critical elements, base and precious metals, to simulate fluid-rock interaction in hydrothermal systems. Recently, the database was augmented with experimental data to accurately model the stability of critical minerals containing rare earth elements such as xenotime and monazite up to 300 °C, and the corresponding aqueous species including the REE^{3+} aqua ions, REE chloride, sulfate, fluoride, and hydroxyl species, with new experimental data available up to supercritical conditions. Here we present applications examples in different geological systems including alteration of basalts and mobility of Te, Pb, Zn, Cu, Au, Ag in VMS deposits, the formation of hydrothermal breccia associated the fluorite, calcite, REE mineralization in critical mineral deposits (carbonatites and alkaline systems), with examples of models that show the type of geochemical and mineralogical data that can be produced for further reactive mass transport modeling that capture fluid flow and reaction paths. Current updates of MINES are supported by DOE BES grant DE-SC0026161 for REE minerals and aqueous species, and NSF CAREER grant EAR-2039674 for modeling natural systems.