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The MINES thermodynamic database for simulating the chemistry of complex crustal fluid-rock systems

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A major problem for predicting the observed rock alteration types and associated metal mobilization in ore forming systems, is the selection of adequate activity models, equations of states and the availability of thermodynamic data for aqueous species, gases and minerals. For this purpose, the open access MINES thermodynamic database (http://tdb.mines.edu) has been recently launched [1] for modeling the chemistry of complex crustal fluid-rock equilibria using the GEM-Selektor program package (http://gems.web.psi.ch).

This database builds on the datasets commonly used for major rock-forming minerals [1,2] and aqueous species from theoretical high P-T predictions [3,4]. The current MINES database and future versions of it, will gradually replace theoretically predicted standard properties of aqueous species with those derived from more recent experimental datasets. Recent efforts [5] have demonstrated a method to reconcile the internal consistency between the minerals and aqueous species databases using the GEMSFITS code for global parameter optimization [6]. These advances, together with the key multicomponent multisite mineral solid solution models and equations of state built in the GEMS codes [7,8], enable us to more accurately model the chemistry of ore forming processes by reactive-transport in higher temperature hydrothermal systems.

The goals behind the MINES database include: i) testing and developing of internally consistent thermodynamic datasets relevant to ore forming processes and crustal metasomatism, ii) expanding our capabilities to model non-ideal solid solutions-fluid equilibria, and iii) promoting and facilitating the use of the GEMS methods and codes [8]. The philosophy of the MINES database is to focus on improving specific thermodynamic datasets by testing a series of modeling projects that can be used to simulate real geological systems. Using the MINES database, I will demonstrate the application of GEM-Selektor to simulate metasomatism of pegmatites and mobilization of REE in the Strange Lake REE-Zr-Nb mineral deposit [9]. I will also demonstrate the coupling of complex chemical equilibria with mass transport along a fluid flow path for simulating the mineralization of Pb and Zn in a Mississippi Valley Type (MVT) deposit [10]. The strategic aim of this research is to stimulate critical evaluation of the open access thermodynamic data among researchers in a community network.

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