A web-based interactive version of SUPCRT92

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Thermodynamic calculations have a long history of applications in geochemistry, and SUPCRT92 (and its predecessors) is one of the most widely used computer codes for performing such calculations [1]. Here, we unveil a new web-based version of the code. SUPCRT92 was originally designed with a dos interface which required either a PC or Linux system, operator knowledge of the reactants included in the database, and operator choice of a set of temperature, pressure or density conditions. Advances in computing power have greatly reduced the amount of time taken to perform thermodynamic calculations. When originally released, SUPCRT92 would take minutes to calculate the thermodynamic properties of a reaction, but with current computer processers calculations take a fraction of a second. Input and output operations are the most time consuming parts of running the original code. In the new web-based version, the interface has been designed to remove barriers and to facilitate an intuitive way for the user to rapidly interact with the program. The web-based version is now available through the GEOPIG website, and is running the slop07 database updated to include thermodynamic data and revised Helgeson-Kirkham-Flowers equation of state parameters published since the last update (slop98). The slop98 database remains an option. In the near future, we expect to greatly expand the number and variety of aqueous organic compounds available for thermodynamic calculations, and the database for the web version will be continuously updated as publications appear.

[1] Johnson et al. (1992) Computers & Geosciences 18(7), 899-947.

Paleorecords of hydrothermal fluid flow and the composition of early Precambrian oceans

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Submarine hydrothermal systems process seawater through infiltration-driven chemical reactions with oceanic crustal rocks. The resulting chemical exchange has been implicated as a control on the composition of the global ocean through time. This relationship is best explored for the Phanerozoic, where high fidelity recorders of changing seawater composition and the chemical anatomy of fossil hydrothermal systems confirm its importance for tracers like O isotopes and Mg:Ca ratios.

For the early Precambrian, isotopic and elemental measurements of seawater proxies suggest an enhanced hydrothermal influence on oceanic constituents like Fe, the REEs, C and S. Accordingly, Precambrian hydrothermal chemical exchange is often treated as a 'black box' whose magnitude is simply increased to drive enhanced cycling of the relevant geochemical tracers. This presentation will be an attempt to open the black box with recent developments from studies of reactive fluid flow and S isotope geochemistry.

Patterns of chemical and isotopic alteration in rocks are paleorecords of the associated reactive fluid flow, and they can be directly inverted for the time-integrated magnitude and geometry of reactive flow systems. Extraction of these fundamental flow characteristics provides a complementary approach for determining the potential impact of hydrothermal systems on the composition of early Precambrian oceans. I will introduce the inverse technique with a Phanerozoic example, and then apply it to select early Precambrian fossil hydrothermal systems.

Combined with a plausible range of flow characteristics, tracer measurements from Precambrian hydrothermal samples can be used to set limits on the composition of coeval seawater. This will be briefly illustrated with a suite of S isotopic measurements of sulfides from the 2.7 Ga Kidd Creek volcanic massive sulfide deposit, Ontario, Canada. The suite exhibits a subdued range of S isotope anomalies relative to the late Archean sedimentary record, indicating the anomaly was not sourced in the hydrothermal system but was transferred through the system as a chemically conservative tracer. The S isotopic dataset reveals a sulfate-poor late Archean marine basin with bottom waters characterized by a complex distribution of reduced S-bearing species.