Development of geochemcial reference materials: USGS experiences and future directions

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Geochemcial Reference Materials (GRMs) are an integral part of any geochemcial program due to their role in methods development, quality control, and instrument calibration. Key aspects to a successful GRM program are to identify current and future needs, produce large quantities of reliable materials and develop new technologies that provide more efficient ways to produce GRMs. Benefiting from the early work of Flanagan and Kane, the USGS has developed a diverse set of 28 powdered reference materials. These materials originally developed to meet USGS programmatic needs have found widespread use in the international community as evidenced by the 12% average annual growth rate in GRM distribution over the past 15 years. Immediate USGS efforts will focus on developing replacements for several of our traditionalGRMs now that their 50 year lifetime is drawing to a close. Work is also planned for the preparation of new materials many in cooperation with outside organizations. The development of a national soil material, synthetic minerals, platinum ore, metalliferous black shale and marine sediment are a few examples.

With expanding interst in trace element microanalysis using Laser Ablation ICP-MS has come a new set of challenges with respoec to the development of calibration and secondary QC materials. A key aspect of this work is the development of microanalytical reference materials (MRMs) that have a wide range of trace elements which are homogeneous at the 10-50 μm spot size. For many geolgic investigations these MRM needs are met through the use of either the MPI-DING, NIST (610, 612, 614) or USGS natural and synthetic basalt glasses. The use of LA-ICP-MS in the analysis of matrices such as coral, bone, sulfides, gems and organic matrices have generated a new urgency for matrix matched MRMs. To meet USGS needs in this area we have developed a series of pressed powders which allow for the quantative analysis of elements in a polymetallic sulfides, carbonates, sulfates, and phosphate matrices.

The development of reference materials will continue to expand but a clearer understanding of what is needed and how best to produce/certify those materials will be important challenges. USGS efforts will focus on development of GRMs and MRMs that are not duplicated by other producers but serve an important role in understanding geological processes on earth and in our solar system.

Thermodynamic estimates for aqueous hydrocarbons

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Aqueous hydrocarbons are involved in geochemical processes at conditions ranging from soils to sedimentary basins to hydrothermal systems. They are metabolized by microbes, transported in fluids, and involved in oxidation-reduction reactions that can be coupled to mineral alteration, gas generation, and transformations of inorganic solutes including metals, as well as sulfur and nitrogen species. Although experimentally determined thermodynamic data are relatively limited, newly developed estimation methods make it possible to greatly expand the number and variety of aqueous hydrocarbons for which calculations are possible. A group estimation method for the thermodynamic properties of hydration of organic compounds [2] permits calculation of standard state properties of aqueous hydrocarbons at the reference temperature and pressure starting with ideal gas data. Corresponding properties at high pressures and temperatures are estimated with a correlation algorithm involving published [3] and newly developed relations among parameters in the revised-HKF equation of state. Estimates for aqueous hydrocarbons were combined with thermodynamic data for liquid hydrocarbons [1] to calculate hydrothermal hydrocarbon solubilities, and the results are in close agreement with experimental solubility data. With nearly 1000 aqueous alkanes, alkenes, and alkynes, as well as cyclic and aromatic hydrocarbons now available for use with SUPCRT92, equilibrium constants for diverse reactions involving hydrocarbons can be calculated over wide-ranging environmental and geologic conditions.

[1] Helgeson *et al*. (1998) *Geochimica Et Cosmochimica Acta* **62**(6), 985–1081. [2] Plyasunov & Shock (2000) *Geochimica et Cosmochimica Acta* **64**(3), 439–468. [3] Plyasunov & Shock (2001) *Geochimica et Cosmochimica Acta* **65**(21), 3879–3900.