Project Title: Aqueous Geochemistry Research

Statement of Problem

The Aqueous Geochemistry Research and Development Project develops and tests new and emerging scientific hypotheses, methods, and modeling applications, and investigates promising research topics in the field of aqueous geochemistry applied to the environmental geochemistry of mineralized areas. New or improved research tools developed within this project will be incorporated into topical projects. This project is divided into four scientific tasks including Modeling Applications and Reaction Pathways, Method Development, Speciation Studies, and Biocatalysis Studies. There is also a scientific task funded through the Toxic Substances Hydrology Program.

The Aqueous Geochemistry Research and Development Project provides a means for researchers to pursue potentially fertile research topics, anticipate and develop new scientific approaches, investigate modeling applications, and develop new or improve current methodologies in the field of aqueous geochemistry. These research efforts will lead to future multi-disciplinary research opportunities and the maintenance of a state-of-the-art aqueous geochemistry research group within the Geologic Discipline. Many projects within the USGS and the Mineral Resources Program rely on low-temperature aqueous geochemistry as an integral part of their study of earth processes. However, development of new aqueous geochemistry approaches, modeling applications, or method development can be a high-risk, long-term activity that is beyond the scope and resources of most topical projects. The Aqueous Geochemistry Research and Development Project affords the opportunity for researchers to develop some of these approaches, applications, and methods, which can then feed back into research efforts in topical projects. The Aqueous Geochemistry Research and Development Project also maintains Mineral Resources Program access to the powerful Geochemist's Workbench suite of computer programs licensed through the University of Illinois.

The overarching theme of the integrated Minerals Environmental Geochemistry projects is to understand, and ultimately to quantify the behavior and distribution of environmentally significant elements as they are dispersed from their sources through the environment. Sources of elements in mineralized terranes include natural and anthropogenic entities, such as ore deposits, their host rocks, mill tailings, and mine waste. Characterization of these source materials involves identifying the mineral phases where the toxic elements reside, the speciation of the toxic elements (e.g., oxidation state and type of bonding to the mineral structure), and the rates and mechanisms of release from the mineral structure. Once released from their sources, physical, chemical, and biological processes act to redistribute and transform dissolved and particulate forms of the elements.

In order to achieve an understanding of these natural systems, the strategy of the integrated Minerals Environmental Geochemistry projects is to conduct interdisciplinary process-oriented studies at scales ranging from molecular to eco-regional, and to develop dynamic models of element cycling that are transferable among environmental systems. The process studies provide the fundamental information for developing conceptual models of the cycling of elements through the environment. Conceptual models synthesize our understanding of element cycling in a given system by identifying the reservoirs of elements (i.e., repositories where elements accumulate or are stored within the system) and the processes that control the amounts of elements in the

reservoirs. The transformation of conceptual models into quantitative, predictive system models requires development of quantitative interrelationships as defined by natural active processes among reservoirs.

Objectives

The objectives of the Aqueous Geochemistry Research and Development Project are 1) to develop and test new and emerging scientific hypotheses, methods, and modeling applications in aqueous geochemistry, 2) to allow pursuit and investigation of promising aqueous geochemistry research topics, 3) to maintain necessary equipment and software for use by a number of researchers, and 4) to provide training in the use and application of aqueous geochemistry methods. Each objective serves to support the integrated objectives, below, for understanding processes and developing models of element cycles in natural and mineralized systems.

The objectives of the integrated Minerals Environmental Geochemistry projects are 1) to advance our understanding of the physical and biogeochemical processes responsible for the mobilization, transport, reaction, and fate of environmentally significant elements (e.g., Al, As, Cd, Cu, Fe, Hg, Mo, Pb, Sb, Se, Zn) in mineralized near-surface systems, and 2) to develop conceptual and quantitative models that link these processes to element distributions and concentrations. This knowledge provides the basis for sound scientific decision making, strategy development, and mitigation activities by local, state, and other federal agencies charged with minimizing the impacts of toxic elements on the environment and biota.

Relevance and Impact

The goal of the Environment and Natural Resources portion of the U.S. Geological Survey Strategic Plan is to "provide science for a changing world in response to present and anticipated needs to expand our understanding of environment and natural resource issues on regional, national, and global scales and enhance predictive/forecast modeling capabilities." In order to achieve this goal, it is necessary to build a strong foundation of fundamental process-oriented research. Many projects within the USGS and the Mineral Resources Program rely on low-temperature environmental and aqueous geochemistry research. Therefore, it is essential to maintain state-of-the-art research capabilities in the field of aqueous geochemistry within the Geologic Discipline. New or improved aqueous geochemistry research tools developed within the Aqueous Geochemistry Research and Development Project will be incorporated into topical projects. These enhanced research capabilities will lead to future multi-disciplinary research opportunities, and will broaden research possibilities for other Mineral Resources Program projects.

Strategy and Approach

The Aqueous Geochemistry Research and Development Project provides a means for researchers to pursue potentially fertile research topics, anticipate and develop new scientific approaches, investigate modeling applications, and develop new or improve current methodologies in the field of aqueous geochemistry. The project is divided into four broad scientific tasks including Modeling Applications and Reaction Pathways, Method Development, Speciation Studies, and Biocatalysis Studies. Each of these tasks incorporates several

activities, and there are built-in synergies between these activities and between the tasks. All of the activities are either outgrowths from topical projects or identified needs from work on topical projects. The Modeling Applications and Reaction Pathways task emphasizes database development, computer-based reaction-path geochemical modeling, computer-based hydrologic fluid-flow modeling, coupled computer-based geochemical/fluid-flow modeling, and laboratory experimental modeling of mineralogically complex systems. The role of the modeling task is to enhance USGS capabilities in the modeling of chemical and physical processes associated with water-rock interactions from ambient to hydrothermal temperatures, and to maintain MRP access to the powerful Geochemist's Workbench suite of computer programs licensed through the University of Illinois. The Method Development task consists of several activities that address the development of geochemical approaches to understanding the chemical and physical processes associated with geochemical cycles and metal mobility. The current focus of the methods task is on isotopic identification of mine waters in ground-water systems, X-ray absorption spectroscopy data-collection methods, use of tracers to evaluate water sources and transport pathways, and studies of natural organic matter/metal complexation. The role of the Speciation Studies task is to investigate and develop state-of-the-art speciation methods for characterization of important constituents in solid and aqueous systems, which will allow better process-level understanding of natural systems and enhance predictive capabilities of the mobility and bioavailability of constituents. Current emphasis of the speciation task is on methods to determine bioavailable metals in aqueous systems, sulfur speciation in solid materials, and metal partitioning reactions between various solid and liquid phases under different geochemical conditions. The Biocatalysis Studies task investigates the role of microbes (primarily bacteria) in the geochemical cycles of arsenic, mercury, iron, lead, and zinc. Activities within the biocatalysis task examine microbial controls on arsenic redox geochemistry, speciation, and mobility, factors that control the rates and pathways of microbial methylmercury production, and the interaction of iron- and sulfur-oxidizing bacteria with mineral surfaces.