Synchrotron XAS Applications in the Real World: The Speciation and Fate of Arsenic and Iron in Natural Sediments

Peggy A. O'Day, *Department of Geological Sciences, Arizona State University*

Friday, September 21, 2001
9:00 am
APS Auditorium

The application of synchrotron-based characterization methods to topics in environmental geochemistry and mineralogy has become a significant research area. A variety of techniques using both hard and soft x-rays are now available to characterize solid, liquid, and gas species, including inorganic, organic, and biochemical entities. One of the more important contributions from these applications has been to “ground truth” the chemical species considered in thermodynamic and kinetic geochemical and biogeochemical models used to describe real environmental systems. Rather than only deducing or guessing the players taking part in reactions, we can select tools to probe for specific elements and obtain chemical information that places constraints on their speciation, structure, and/or spatial distribution.

While new synchrotron methods continue to develop, several methods useful for environmental systems have become fairly routine, in particular, x-ray absorption spectroscopy or XAS (x-ray absorption near-edge structure [XANES] and extended x-ray absorption fine structure), powder and micro x-ray diffraction, and micro x-ray fluorescence. As such, they can be integrated with more traditional geochemical and physical analyses to contribute to the overall understanding of reaction and transport in complex natural systems. Examination of redox-sensitive metals in soils, sediments, and water is particularly amenable to analysis by XAS because solid, aqueous, and adsorbed species can be probed and changes in oxidation state readily observed in XANES spectra. This talk will present several examples of how XAS information was used to constrain the speciation of iron, arsenic, and other metals at contaminated sites and in laboratory simulation experiments. When combined with chemical and physical characterizations of sediments and porewater, these data are used to: (1) directly assess the extent of heterogeneous equilibrium among species predicted by thermodynamic modeling, (2) determine iron availability and field rates of Fe(III) reduction and pyritization in reduced estuary sediments, (3) examine the attenuation of arsenic as a function of the rate and extent of arsenic oxidation in unsaturated and saturated shallow subsurface sediments, and (4) verify the speciation of reactants and products in laboratory experiments designed to assess remediation and contaminant removal methods for arsenic. These examples lend insight into cycling processes for iron and arsenic under conditions of low and high dissolved sulfate across oxic/anoxic boundaries.