

Argonne Subsurface Science Program SFA

Argonne National Laboratory
Subsurface Science Scientific Focus Area (SFA)

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EXECUTIVE SUMMARY

Argonne Subsurface Science Program Scientific Focus Area (SFA) integrates synchrotron-based biogeochemistry with microbiology, molecular biology, and protein biochemistry to pursue the long-term scientific objective of elucidating the molecular basis of the interplay between specific microbial metabolic activities, solution chemistry, and mineralogy contributing to the transformations of contaminants at DOE field sites. To pursue this scientific objective, specific hypotheses are tested by capitalizing on unique Argonne capabilities together with key collaborative efforts at other National Laboratories and academic institutions. The scientific objectives of this SFA drive the development and optimization of synchrotron methods for measurements at the molecular level pertinent to understanding contaminant transformations in subsurface environments. The current over-arching concept driving the Argonne Subsurface Science program is that *microbial metabolic activity — together with changes in Solution chemistry, mineralogy, and solid phase surface reactivity, and the presence of electron donors, acceptors and shuttles — affects the distribution of (bio)mineral phases, as well as the rate, extent, and mechanisms of contaminant transformation.*

To address this concept, the proposed 5-year research plan involves the integration of microbiology, molecular biology, protein biochemistry, geochemistry, and physics to characterize the transformation of the contaminants uranium and mercury. Experiments are proposed, to be done at Argonne with collaborators from Pacific Northwest National Laboratory (PNNL), Oak Ridge National Laboratory (ORNL), Michigan State University, University of Iowa, University of Illinois Urbana Champaign, Stanford University, Hamilton College, Northeastern University, University of Sofia, and the Illinois Institute of Technology, to (1) determine what aspects of microbial activity, solution chemistry, and Fe(III) mineralogy are key to the distribution of Fe(II) species resulting from dissimilarity iron reduction, (2) evaluate the reactivity of biogenic Fe(II) phases with respect to the transformation of redox active contaminants, with an emphasis on understanding the kinetics and mechanisms of the transformation of U(VI) and Hg(II), (3) characterize the contaminant transformations at the molecular level using a range of synchrotron approaches, and (4) investigate the role of microbial and mineral surfaces, microbial biofilms, and exuded microbial polymers on electron transfer, surface sorption, and surface precipitation mechanisms as they relate to their effects on the chemical speciation and mobility of U(VI) and Hg(II). Initial experimental work will be focused on *Anaeromyxobacter* spp., *Geobacter* spp., and microbial consortia from the ORNL, UMTRA, and PNNL IFCs.

The experimental work of the Argonne Subsurface Science SFA will drive technological development at Advanced Photon Source beamlines to provide the needed synchrotron measurements. These developments will include (1) optimization of x-ray fluorescence micro(spectro)scopy capabilities (~1-100 micron spatial resolution) at the MRCAT/EnviroCAT

insertion device beam line, (2) development and standardization of x-ray fluorescence nano(spectro)scopy (~10-100 nm spatial resolution) capabilities at the XOR sector 2 insertion device beam line, (3) development of the First Optical Enclosure (FOE) of the MRCAT/EnviroCAT bending magnet beam line, followed by the development and buildout of an experimental hutch at the MRCAT/EnviroCAT bending magnet beam line, dedicated to bulk x-ray absorption fine structure spectroscopy, (4) development of synchrotron-based hard x-ray capabilities for *in-situ* investigations of coupled microbiological and geochemical processes within static and free-flowing microcosm columns, (5) development of high-throughput approaches for xray micro(spectro)scopy experiments, and (6) integration of newly-developed x-ray microscopy techniques with electron microscopy techniques for investigations of mineral-metal-microbe interactions.