U.S. Department of Energy
Office of Science

Office of Biological and Environmental Research
Climate and Environmental Sciences Division

Subsurface Biogeochemical Research Strategic Plan

Leading to a holistic understanding of subsurface environmental processes applicable to a range of DOE energy and environmental challenges.

June 2010

Contents

DOE Office of Biological & Environmental Research: Subsurface Biogeochemical Research (SBR)

I. Current Situation

The subsurface environment, which encompasses the vadose and saturated zones, is a heterogeneous, geologically complex domain. Believed to contain a large percentage of Earth's biomass in the form of microorganisms, the subsurface is a dynamic zone where important biogeochemical cycles work to sustain life. Actively linked to the atmosphere and biosphere through the hydrologic and carbon cycles, the subsurface serves as a storage location for much of Earth's fresh water. Coupled hydrological, microbiological, and geochemical processes occurring within the subsurface environment cause the local and regional natural chemical fluxes that govern water quality. These processes play a vital role in the formation of soil, economically important fossil fuels, mineral deposits, and other natural resources.

Cleaning up Department of Energy (DOE) lands impacted by legacy wastes and using the subsurface for carbon sequestration or nuclear waste isolation require a firm understanding of these processes and the documented means to characterize the vertical and spatial distribution of subsurface properties directing water, nutrient, and contaminant flows. This information, along with credible, predictive models that integrate hydrological, microbiological, and geochemical knowledge over a range of scales, is needed to forecast the sustainability of subsurface water systems and to devise ways to manage and manipulate dynamic *in situ* processes for beneficial outcomes.

Predictive models provide the context for knowledge integration. They are the primary tools for forecasting the evolving geochemistry or microbial ecology of groundwater under various scenarios and for assessing and optimizing the potential effectiveness of proposed approaches to carbon sequestration, waste isolation, or environmental remediation. An iterative approach of modeling and experimentation can reveal powerful insights into the behavior of subsurface systems. State-of-science understanding codified in models can provide a basis for testing hypotheses, guiding experiment design, integrating scientific knowledge on multiple environmental systems into a common framework, and translating this information to support informed decision making and policies.

The Subsurface Biogeochemical Research (SBR) activity within the Office of Biological and Environmental Research (BER) is advancing a basic understanding of subsurface processes at the intersection of biology, chemistry and physics. SBR supports interdisciplinary research in an iterative cycle of hypothesis generation, experimentation and modeling between the laboratory and the field. The current focus of the SBR is on the understanding of processes impacting the mobility of contaminant metals and radionuclides found in the subsurface at DOE legacy waste sites but the overall scientific approach is applicable to a wide range of DOE relevant energy and environmental challenges including:

- Cleanup of contaminants and stewardship of former weapons production sites
- Underground storage of spent nuclear fuel
- Carbon cycling and sequestration in the environment

- Nutrient cycling in the environment in support of sustainable biofuel development
- Fossil fuel processing and recovery from the deep subsurface.

Science-based understanding and solutions to these challenges are constrained by:

- The inherent complexity and inaccessibility of subsurface environments and the strong coupling of biological, chemical and physical processes across vast spatial and temporal scales.
- Lack of well established holistic approaches for understanding, predicting and controlling biogeochemical and hydrodynamic processes in realistically complex subsurface environments.

II. Inputs & Resources

SBR supports interdisciplinary approaches to understanding environmental processes. The approach couples hypothesis testing with experiment, observation and modeling in an iterative cycle to enhance the understanding of coupled of biological, physical and chemical processes occurring across scales in subsurface environments applicable to DOE energy and environmental challenges. This research is performed by:

- Integrated research programs (Scientific Focus Area) at the DOE National Laboratories
- University researchers with multidisciplinary capabilities
- University-based "Exploratory" research for new concepts and investigators
- Integrated Field Research Challenge (IFRC) sites

SBR advances a fundamental understanding of environmental processes at the intersection of biology, chemistry and physics and is heavily leveraged with a unique combination of BER programs and DOE user facilities including:

- Genomic sciences research
- Terrestrial carbon cycle research
- Ecosystem research
- Environmental Molecular Science Laboratory (EMSL)
- Joint Genome Institute (JGI)
- Synchrotron light sources

Additionally, SBR research is leveraged with other programs offices within the Office of Science including:

- Office of Advanced Scientific Computing Research (ASCR) via the SciDAC program (Scientific Discovery through Advanced Computing)
- Office of Basic Energy Sciences (BES), Geosciences program

Internal DOE and external programs that are either complementary to SBR research and/or actively leverage off of SBR-funded research include:

- SERDP (Strategic Environmental Research and Development Program)
- ASCEM (Advanced Scientific Computing for Environmental Management)

SBR research addresses environmental challenges of relevance to several DOE offices including:

- Office of Environmental Management (Groundwater and Soil Remediation)
- Office of Legacy Management
- Office of Fossil Energy (National Energy Technology Laboratory, NETL)

III. Near Term Goals (1-3 Years):

- *Develop interdisciplinary approaches to describe the coupling of biological, physical and chemical processes.*

  Coordinated interdisciplinary approaches that iterate between the laboratory and the field are needed to understand the complex coupling of biological, physical and chemical processes occurring in subsurface environments.

- *Build on advances in genome-enabled science and incorporate a mechanistic understanding of microbial activity into the understanding of environmental processes.*

  Current descriptions of microbial activity in environmental process models are limited in predictive power due to an inadequate understanding of how microorganisms function in the environment. SBR research is leveraging off advances in the genomic sciences pioneered within BER programs and further developing a more mechanistic understanding of microbial communities and how their activity is coupled to and affected by environmental process. A mechanistic approach to the understanding of microbial activity afforded by genome-enabled systems approaches to cellular metabolism will provide a more realistic understanding of microbial functioning in the environment of interest to DOE.

- *Improve the understanding of the geochemical form, stability, speciation and rates of transformation of minerals in environmental processes.*

  Mineral transformation either via chemical or biological means is an important component of subsurface biogeochemical processes influencing the mobility of contaminants, carbon/nutrient forms and the geochemical character of groundwater. Reactive transport models require a detailed understanding of mineral composition and transformations to realistically track changes in subsurface processes impacting contaminant, carbon and nutrient mobility.

- *Develop innovative methods for characterizing and monitoring biogeochemical and hydrologic responses.*

Innovative methods are needed to evaluate the heterogeneous nature of subsurface environments and processes. New geophysical and environmental monitoring (i.e. tracer) methods are needed to detect and measure biogeochemical processes to more fully understand the space/time dependence of environmental processes.

- *Develop computational models of coupled biogeochemical and hydrodynamic processes.*

  Predictive models provide the context for knowledge integration and are the primary tool to forecast the evolving geochemistry or microbial ecology of groundwater under various scenarios; or to assess and optimize the potential effectiveness of a sequestration, isolation, or proposed remediation approach. An iterative approach of modeling and experimentation can provide powerful insights on the behavior of subsurface systems.

- *Explore approaches to manipulate and control biogeochemical processes in the environment.*

  Implicit in several of DOE's energy and environmental challenges is a need to explore ways to manipulate and/or control biogeochemical processes in the environment to some beneficial end. New approaches are needed to address environmental contamination, carbon sequestration, and contingency planning for future nuclear material storage. Similar new approaches are needed for nutrient management strategies and recovery of residual fossil fuels from the deeper subsurface.

IV. Mid Term Goals (3-6 Years):

- *Incorporate new metabolic modeling strategies and approaches to measuring microbial activity in the environment into coupled reactive transport models.*

  Advances in genome science continue to provide a more mechanistic and quantitative understanding of cellular metabolism. This understanding is increasingly being incorporated into new mechanistic models of microbial physiology. SBR will continue to advance genome-enabled studies of environmentally relevant microorganisms and microbial communities and incorporate new metabolic models of microbial metabolism into reactive transport models of environmental processes and test predictions. SBR will also develop new approaches and methods to measure microbial activity and validate genome-based metabolic models in environmental systems.

- *Incorporate new geochemical and molecular-scale understanding of biologically-mediated mineral transformations, including kinetics, into coupled reactive transport models.*

Reactions occurring at the mineral-water and microbe-mineral interface control the composition of water in subsurface environments. Predicting the evolution of water composition in the environment requires a fundamental understanding of mineral composition, transformation and rates of reactions. SBR will continue to advance new geochemical, biogeochemical and kinetic studies of mineral-microbe-water interactions leveraged by capabilities at EMSL and the synchrotron light sources. These detailed studies will be incorporated into reactive transport models to test and refine predictions of environmental processes.

- *Incorporate methods for characterizing and monitoring biogeochemical and hydrologic responses at different spatial and temporal scales into reactive transport models.*

  The subsurface environment is complex and heterogeneous yet our current descriptions of these processes are simplistic and homogeneous. New approaches are needed to characterize and monitor the heterogeneous distribution of biogeochemical processes in subsurface environments across broader spatial scales and with higher spatial and temporal resolution to better understand the structure and function of subsurface environmental systems.

- *Develop computational approaches to predictive modeling, linking multiple environmental processes at different spatial and temporal scales.*

  SBR conducts research on a wide variety of biogeochemical processes at a variety of observational scales ranging from molecular to field scales. Incorporating and linking diverse data obtained from a variety of scales is a challenging computational problem. New methods are needed to understand and translate information on environmental processes derived at smaller scales to processes occurring at broader spatial/temporal scales. Simplification methods and/or scaling methods that accurately capture the influence of smaller scale processes on larger scale observations are critical to predicting many of the biogeochemical processes of relevant to DOE's energy and environmental challenges.

- *Iteratively refine the performance of numerical models in hypothesis-driven, manipulative experiments of environmental processes.*

  Models are an integral component of SBR rather than an end product of the research. Incorporation of new biological, geochemical and geophysical information into reactive transport models leads to new hypotheses for research. The SBR emphasis on iterative research coupling hypothesis testing with experiment, observation and modeling implies that models of environmental processes be continuously tested via manipulative experiments to refine model performance. These experiments synthesize and holistically test information obtained on varied biological, geochemical and hydrologic processes active in subsurface environments. The testing is crucial to demonstrating understanding of environmental processes and refining the accuracy of model predictions.

V. Long Term Goals (7-10 Years):

- *Develop fully coupled models of subsurface environmental processes that incorporate: metabolic modeling of microbial processes; molecular-scale understanding of geochemical stability, speciation and biogeochemical reaction kinetics; and diagnostic signatures of the system response at varying spatial and temporal scales.*

  A holistic understanding of subsurface biogeochemical processes is the goal of SBR. A result of the repeated pattern of interdisciplinary, iterative hypothesis testing with experiment, observation and modeling is state-of-science understanding codified in models. Fully coupled models of subsurface processes that can predict the behavior of environmental processes across a range of spatial and temporal scales will provide a framework for integrating scientific knowledge on environmental systems and for translating this information for use in decision making and policy.

- *Develop integrated approaches to test model predictions and to identify and reduce sources of prediction uncertainty (e.g., model formulation and parameterization)*

  As models become more complex there is a need to develop new approaches to test model predictions and identify sources of uncertainty. Increasingly, models of environmental processes are required to be accompanied by an assessment of the uncertainty of the model predictions. New methods are needed to test for deficiencies in understanding and assess sources of uncertainty in model predictions.

- *Test strategies to predict, manipulate and control subsurface biogeochemical processes in key subsurface environments to address DOE's energy and environmental challenges.*

  The development of fully coupled models capable of describing complex environmental processes could be used to help design, test and/or simulate manipulative processes addressing DOE's energy and environmental challenges. Ideally, these models would be used in concert with an experimental approach that fully incorporates model predictions into the process design with monitoring methods that feedback environmental process information to refine model projections.

VI. Impact: Positive Outcomes for Science and Society

The SBR approach leads to a holistic understanding of subsurface environmental processes applicable to a range of DOE energy and environmental challenges. The emphasis on iterative, interdisciplinary experimental research in concert with modeling and monitoring approaches will lead to:

- *Increased understanding of coupled biogeochemical processes in key subsurface environments that enable system-level prediction and control.*
- *Robust strategies to monitor, immobilize or remove former weapons production-related contaminants from the environment.*
- *Science-based approaches to risk assessments of spent nuclear fuel storage.*
- *Strategies for carbon sequestration (both deep subsurface and terrestrial) and reducing climate model uncertainly in predicting the biogeochemical cycling of carbon in soils and sediments.*
- *Improved understanding of coupled plant-microbe-mineral interactions controlling nutrient cycling in soils to aid development of sustainable biofuels.*
- *Strategies for manipulating deep subsurface biogeochemical processes to enhance fossil fuel processing and recovery.*
- *Reduced risk and cost of managing subsurface environmental and energy systems and increase public acceptance.*