Scientific Understanding Enables U.S. Water and Energy Security

The Subsurface Biogeochemical Research (SBR) program within the U.S. Department of Energy’s (DOE) Office of Biological and Environmental Research is strategically aligned with DOE’s mission to ensure U.S. security and prosperity through watershed system science. Water resources critical for energy production are under pressure from growing water demand, contamination, drought, flooding, and saltwater intrusion. Sustainable management of watershed systems and their coupling with the built environment rely on understanding the hydrological and biogeochemical processes that control watershed system dynamics and water availability and quality. Next-generation science-based models of watershed systems are needed to address many U.S. energy and environmental challenges, including contaminant cleanup, clean water availability, safe storage of energy and nuclear byproducts in the subsurface, nutrient availability for sustainable biofuel crops, and recovery of subsurface energy resources.

Priority Research Objectives

SBR has five Priority Research Objectives that build upon foundational SBR workshops (doesbr.org/program/pubs.shtml), use a network of SBR-supported watershed testbeds within the contiguous United States, and set the stage for advancing watershed system science for energy over the next decade. Addressing these objectives requires the systems-level approaches and perspectives that are hallmarks of SBR research.

1. Quantify how biological behavior, abiotic-biotic interactions, and molecular transformations control the mobility of contaminants (e.g., U, Tc, Hg), nutrients (e.g., N, P, C), and critical biogeochemical elements (e.g., S, Fe, Mn).
2. Quantify and predict how hydrology drives fine-scale biogeochemical processes in surface-subsurface systems.
3. Translate biogeochemical behavior across relevant molecular to watershed scales to accurately and tractably predict flows of water, nutrients, and contaminants.
4. Identify, quantify, and predict watershed responses to natural and anthropogenic perturbations and shifts to new states.
5. Translate predictive understanding of watershed system function and evolution into near- and long-term environmental and energy strategies.
Scientists seek to determine how perturbations to mountainous watersheds (e.g., floods, drought, and early snowmelt) affect the downstream delivery of water, nutrients, carbon, and metals over seasonal to decadal timescales through the development and testing of scale-adaptive modeling. [Courtesy LBNL]

Predictive Understanding of Hydrobiogeochemical Dynamics

The overarching objective of SBR is to advance a robust, predictive understanding of how watersheds function as integrated hydrobiogeochemical systems and how these systems respond to perturbations. Example perturbations include changes in weather patterns, extremes, land use, water management, vegetation cover, snowmelt timing, and contaminant release. Through tight iteration among observations, experiments, and modeling, SBR obtains a systems-level understanding of how watersheds function. Understanding system function requires examining how surface and subsurface water flow and constituents are transported over a broad range of spatiotemporal scales and how biogeochemical processes mediated by microorganisms enable mineral dissolution and precipitation, organic matter deposition and degradation, oxidation and reduction reactions, and plant-rhizosphere interactions.

SBR’s integrated approach is particularly important for assessing and managing the full extent of challenges posed by DOE’s persistent and dynamic subsurface contamination challenges. For example, an integrated perspective of the watershed system is critical for both designing cost-effective remediation strategies based on knowledge of contaminant fate and transport and for predicting watershed resilience to floods, droughts, heat waves, and compounding extremes. Significant fundamental knowledge gaps impede current watershed models from predicting system dynamics and evolution with the confidence required to address pressing U.S. energy and environmental challenges. Decades of SBR research in subsurface and watershed system science have produced world-leading capabilities and expertise, as well as a vast number of discoveries and impacts in multiple scientific fields (see Recent SBR Discoveries and Accomplishments).

Recent SBR Discoveries and Accomplishments*

- Simulation of watershed system behavior across continental scales to demonstrate that groundwater flow plays a significant role in evapotranspiration.
- Hydrogeophysical methodologies used to characterize subsurface microbial activity.
- Immobilization of uranium and chromium in groundwater using microorganisms.
- Discovery of mercury methylation genes that regulate ecosystem-scale mercury transport.
- Discovery and elucidation of ecosystem hot spot and hot moment controls over fluxes and bioavailability of contaminants, nutrients, and critical elements.
- Development and use of genome-informed reactive transport modeling capability.
- Integrated molecular- through watershed-scale hydrobiogeochemical models to predict long-term plume behavior.
- Significant expansion of the known microbial “tree of life” through subsurface metagenomic analyses.
- Identification of the lower size limit of a living cell.
- Demonstration of the importance of metabolic handoffs in nutrient cycling across surface-subsurface systems.

* Expanded list and citations provided at doesbr.org/program/benefits.shtml
Research Activities and Enabling Resources

To address the Priority Research Objectives, SBR supports six Scientific Focus Areas (SFAs), university-led research projects, a community cyberinfrastructure, and educational and outreach resources.

**SBR SFAs (doesbr.org/research/sfa/).** Carried out within distributed watersheds, the six SFAs represent a network of **complementary testbeds** for tackling a range of DOE energy and environmental challenges.

- **Watershed Function SFA, LBNL** — Developing new insights and scale-aware approaches to predict how mountainous watersheds retain and release water, nutrients, carbon, and metals and respond to perturbations over episodic through decadal timescales (watershed.lbl.gov).

- **River Corridor and Watershed Hydrobiogeochemistry SFA, PNNL** — Quantifying and predicting hydrobiogeochemical and ecological impacts of hydrologic exchange between subsurface and river environments, particularly in hydropower-impacted, highly managed systems (sbrsfa.pnnl.gov).

- **Biogeochemical Transformations at Critical Interfaces SFA, ORNL** — Determining the fundamental mechanisms and environmental factors that control mercury biogeochemical transformations at key interfaces in terrestrial and aquatic ecosystems (www.esd.ornl.gov/programs/rsfa/).

- **Groundwater Quality SFA, SLAC** — Quantifying and modeling mechanisms by which fine-scale biogeochemical and transport processes in shallow alluvial aquifers couple to one another and control water quality under hydrologically variable conditions. Molecular- to meter-scale process models support SBR watershed-scale research (ssrl.slac.stanford.edu/sfa/).

- **Subsurface Biogeochemistry of Actinides SFA, LLNL** — Advancing the understanding of subsurface actinide
River Corridor and Watershed Biogeochemistry. Installation of an aquifer tube to monitor the hydrologic exchange of river water and groundwater and associated biogeochemical processes in the Hanford Reach of the Columbia River. This tube and several others are concurrently monitored using geophysical methods for three-dimensional characterization of hydrologic exchange under varying river conditions, water sampling for biogeochemical analyses, and assessment of temperature and other water quality variables. [Courtesy PNNL]

behavior from the molecular to field scale to provide a scientific basis for remediation and long-term stewardship of groundwater quality at DOE legacy sites (doesbr.org/research/sfa/sfa_lnl.shtml).

- **Iron and Sulfur Biogeochemistry in Redox Dynamic Environments SFA, ANL** — Elucidating the molecular-to-meter-scale interplay among microbial processes, solution chemistry, and mineralogy contributing to the mobility of elements and contaminants in hydrologically dynamic systems (doesbr.org/research/sfa/sfa_anl.shtml).

**University-Led Research Projects.** SBR supports a diverse portfolio of projects led by university principal investigators (doesbr.org/research/university.shtml). This fundamental research uses integrative, hypothesis-driven approaches to examine critical subsurface biogeochemical, hydrobiogeochemical, and ecohydrological processes in studies that complement, but not duplicate, SFA activities.

**Community Cyberinfrastructure.** SBR advances an open-source computational simulation and data science infrastructure to enable integration of multiscale, multiphysics models with diverse and complex environmental datasets. These models capture with high fidelity the hydrobiogeochemical structure and function of watershed systems, enabling DOE to address future energy and environmental challenges.

Key components of SBR’s cyberinfrastructure include the Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) and Interoperable Design of Extreme-scale Application Software (IDEAS) project. ESS-DIVE is an archive for observational, experimental, and modeling data gleaned from DOE-supported terrestrial and subsurface ecosystem research. The IDEAS project is creating an extreme-scale scientific software development ecosystem composed of high-quality, reusable computational science and engineering software components and libraries; a collection of best practices, processes, and tools; and substantial outreach mechanisms for promoting and disseminating productivity improvements.

**Education and Outreach.** SBR is a premier resource for educating the next generation of scientists to use experimental, observational, and modeling to study and advance understanding of how watershed systems function across a vast range of temporal and spatial scales.

**Biogeochemical “Hot Moments.”** Researchers installed in situ, permeable solid phase-groundwater reaction cells into wells at DOE’s Rifle, Colorado, field site to investigate molecular-scale mechanisms governing uranium mobility in response to seasonally changing groundwater conditions. This work showed that transiently high dissolved oxygen concentrations, occurring in late spring during meltwater runoff, created biogeochemical “hot moments” that dominated oxidative mobilization of uranium for the entire year. [Courtesy SLAC]

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