LBNL Sustainable Systems SFA

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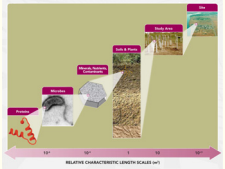
http://esd.lbl.gov/research/projects/sustainable_systems/

INTRODUCTION

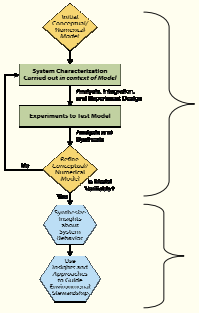
The LBNL Sustainable Systems SFA addresses critical knowledge gaps associated with environmental stewardship of metals and radionuclides in the subsurface.



Our research is motivated by the recognition that active remediation and natural attenuation strategies for persistent radionuclides and metals (a) are governed by complex, scale-dependent, and often coupled hydrological, geochemical and microbiological subsurface processes and (b) must be compatible with hydrobiogeochemical conditions that prevail in their immediate environment to be sustainable over stewardship time frames.

The overarching premise of our Sustainable Systems SFA is that improvements in the mechanistic connections between fundamental hydrobiogeochemical processes and their macroscopic manifestations are needed to guide sustainable environmental stewardship in the complex subsurface.

Our research is being performed within a Systems Framework, where complex subsurface systems hypotheses are tested through consideration of the nature and interaction of key hydrological, microbiological, and/or geochemical components.



Systems Framework: Conceptual/Numerical Model that considers the nature and interactions of key system components as needed to mechanistically connect fundamental processes with overall system behavior

Outcomes: Improved understanding of system behavior as needed to guide sustainable stewardship

We have defined **three Challenges** that are allowing us to test the benefits of the Systems Framework across multiple scales:

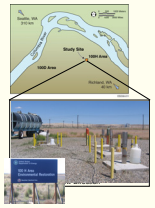
1) Unraveling Biogeochemical Reaction Networks
2) Evolution of Pore Structures and Flowpaths
3) Predicting Contaminant Mobility

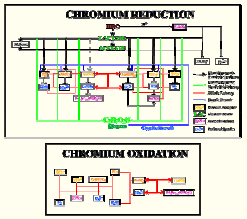
The defined challenges are being performed by multi-disciplinary research teams at three DOE relevant field sites. The challenges are addressing complex, multi-scale subsurface problems and are utilizing LBNL's expertise in investigative methods that **span the molecular to the field scales**.

UNRAVELING BIOGEOCHEMICAL REACTION NETWORKS CHALLENGE

Motivation

This Challenge focuses on characterizing interrelated microbial metabolic and geochemical mechanisms and rates associated with Cr(VI) biostimulation and reoxidation as needed to assess long-term sustainability of Cr(VI) biostimulation. This challenge builds on previous LBNL-led research that demonstrated the ability of bioremediation to reduce Cr(VI) below drinking water standards at the Hanford 100H Site in the vicinity of the injection well for several years (Faybishenko et al., 2008). Although the previous research indicated the potential of bioremediation for Cr(VI) reduction, several questions remain about the associated pathways and sustainability of the approach, which form the basis for the hypotheses in this Challenge.



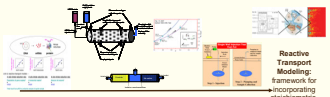


Hypotheses

1. Microbial processes mediate both **direct (enzymatic) and indirect Cr(VI) reductions** at Hanford 100H, but indirect pathways dominate sustained reduction.
2. The **rate and extent of Cr(III) (re)oxidation** will be controlled by the abundance and mineral form of Mn (III/IV) oxides in the sediment.
3. Fermentative/acetogenic versus respiratory metabolism will promote **retention of organic carbon in the aquifer.**

Approaches

The three hypotheses are being carried out via interrelated tasks using biomolecular, spectroscopic, isotopic, and reactive transport modeling approaches. The tasks are being carried out from the molecular to the local (push-pull) field scale, as is needed to assess long-term sustainability of chromium bioremediation.



Biomolecular signatures: Elucidate reaction pathways by studying microbial gene expression at the community level

Column Studies: To explore mechanisms and signatures under controlled conditions

Spectroscopic Signatures: Quantify chemical mechanisms and microbe-mineral interactions

Isotopic Signatures to quantify key redox state, nutrient availability, and microorganisms involved.

Push-Pull tests to test hypotheses at field scale in collaboration with GIL

Reactive Transport Modeling: framework for incorporating stoichiometric, isotopic, and biomolecular information as needed to test pathway hypotheses and to predict Cr(VI) bioreduction sustainability

Nominal Team: Harry Beller, Eoin Brodie, John Christensen, Mark Conrad, Boris Faybishenko, Terry Hazen, Peter Nico, Eric Sonnenthal, and Carl Steefel.

Key Collaborators: Arkin/Hazen Genomes to Life Stress Project and Mike Truex (PNNL)

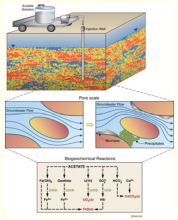
Visit other Posters:

•Beller et al., Use of biomolecular signatures to unravel biogeochemical reaction networks underlying chromium reduction at the Hanford 100H site.
•Hazen et al., Field-Scale Investigations of Cryptic Growth and Memory Response Hypotheses at the Chromium Contaminated Hanford 100-H Site.
•Steefel et al., Reactive Transport Modeling of Microbially-Mediated Processes at the Old Rifle and Hanford 100H Sites

EVOLUTION OF PORE STRUCTURES AND FLOWPATHS CHALLENGE

Motivation

This Challenge focuses on development of a predictive understanding of how remediation-induced biogeochemical transformations modify the connectivity of the pore structure and how those changes are manifested at the field scale, as is needed to design, execute, and interpret sustainable in situ treatments. The Challenge research is motivated by the recognition that feedbacks between flow characteristics and biogeochemical transformations are not well understood and by recent LBNL-led research at the DOE Rifle IFRC site that indicated that flow properties were modified during field-scale Uranium bioremediation (Englert et al, 2008; Li Li et al., 2009).

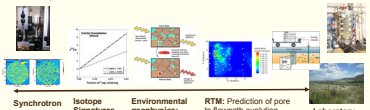


Hypotheses

1. Remediation treatments can induce significant enough biogeochemical perturbations to **alter pore structures**
2. The cumulative impact of remediation-induced biogeochemical transformations will be significant enough to **impact flowpaths at the field scale**.
3. The dynamic nature of field-scale flowpaths will impact the efficacy and **sustainability of *in-situ* remediation treatments**.

Approaches

The three hypotheses are being carried out via integrated tasks using synchrotron, isotopic, geophysical, and reactive transport modeling approaches, which are being tested at the uranium-contaminated Rifle, Colorado IFRC site.



Synchrotron dynamic investigations of pore structure evolution and chemical trans-formations

Isotope Signatures of the onset and extent of sulfate reduction and calcite precipitation during bio-stimulation

Environmental geophysics: remote monitoring and estimation of precipitate evolution.

RTM: Prediction of pore to flowpath evolution, feedbacks, and impact on sustained remediation

Laboratory and Field Studies tied to Rifle IFC Big Rusty Site

Nominal Team: Jonathan Ajo-Franklin, Jinsong Chen, Mark Conrad, Don DePaolo, Stefan Finsterle, Li Li, Susan Hubbard, Peter Nico, Ken Williams, Yuxin Wu.

Key Collaborators: Phil Long (PNNL) and the Rifle IFC Team

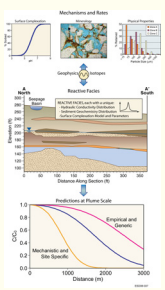
Visit other Posters:

•Nico and Ajo-Franklin, Dynamic Synchrotron Imaging of Pore Structure Evolution
•Druhan et al., Isotopic signatures for key mineralogical reactions accompanying biostimulated uranium reduction
•Hubbard et al., Quantification of Hydrogeological Controls and Induced Biogeophysical Transformations associated with In-Situ Bioremediation using Geophysical Methods
•Steefel et al., Reactive Transport Modeling of Microbially-Mediated Processes at the Old Rifle and Hanford 100H Sites

PREDICTING CONTAMINANT MOBILITY CHALLENGE

Motivation

This Challenge is motivated by the recognition that predictions of contaminant evolution, migration, and remediation efficacy at the plume scale often fail because of the great simplifications that are typically made in the representation of subsurface heterogeneity and coupled hydrobiogeochemical processes. This gap hinders our ability to guide sustainable stewardship of many DOE plumes.



Hypotheses

1. A limited number of sediment groups can be defined that individually display unique **U and Sr sorption/precipitation processes** and that adequately represent the spectrum of geochemical behavior in the subsurface when considered as an ensemble.
2. Reactive transport properties and mechanisms can be tractably characterized using a "**reactive facies**" concept.
3. An optimal level of **model complexity for prediction of contaminant** mobility at the plume scale can be identified, beyond which model accuracy does not increase significantly.

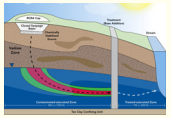
Approaches

•This Challenge explores the utility of an organizing principle to integrate laboratory-obtained information about rates and mechanisms with field-based hydrogeological characterization, as is needed to make reliable and computationally tractable predictions of plume evolution.

•The Challenge includes a formal evaluation of the benefit of increasing complexity on successful predictions of contaminant mobility over stewardship time frames.

•The research is carried out through integrated laboratory geochemical experiments; synchrotron, isotopic, and geophysical characterization, and reactive transport modeling.

•The insights and methods developed in this challenge will ultimately be used to assess the natural attenuation capacity of the acidic, uranium and strontium plumes of the Savannah River Site F-Area.



Nominal Team: John Christensen, Susan Hubbard, Mike Kowalsky, Peter Nico, Sudipta Rakshit, Nic Spycher, Carl Steefel, and Jiamin Wan.

Key Collaborators: The project is being performed in collaboration with EM-supported SRNL scientists led by Miles Denham.

Visit other Poster:
Spycher et al., Predicting Plume-Scale U and 90Sr Mobility at the Savannah River Site

EXPLORATORY PROJECTS

The LBNL SFA also includes several Exploratory Projects that are investigating critical Sustainable System aspects. Please also **visit these exploratory project posters**:
•Conrad et al., Enhanced Immobilization of Metals and Radionuclides in the Vadose Zone
•Tokunaga et al., Uranium Immobilization in Oxidizing Environments: Potassium Uranyl Vanadate Precipitation

ERSP ANNUAL PI MEETING APRIL 20-23, 2009

Funding for this study was provided by the U.S. Department of Energy, BER Program Contract DE-AC020SCH11231 to the LBNL Sustainable Systems Scientific Focus Area