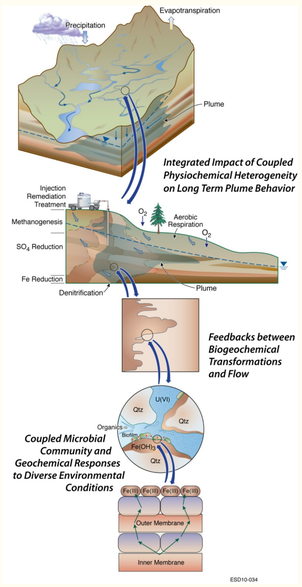
SUSTAINABLE SYSTEM SCIENTIFIC FOCUS AREA

Susan Hubbard (LRM; sshubbard@lbl.gov), Harry Beller, Jim Davis, Carl Steefel, Ken Williams
Jonathan Ajo-Franklin, Eoin Brodie, Romy Chakraborty, Jinsong Chen, John Christensen, Mark Conrad, Miles Denham (SRNL), Wenming Dong, Don DePaolo, Boris Faybishenko, Yoshiko Fujita (INL), Jim Hunt (UCB), Michael Kowalsky, Li Li (Penn State), Peter Nico, Dimitris Silin, Eric Sonnenthal, Nic Spycher, Tetsu Tokunaga, Jiamin Wan,Li Yang, Yuxin Wu
(all LBNL except where noted)

INTRODUCTION



The overarching mission of the Sustainable Systems SFA is to improve the predictive understanding of subsurface flow and transport relevant to metal and radionuclide remediation and long-term environmental stewardship.

The SFA is composted of **three key challenges**, targeted to address current obstacles for developing a predictive understanding of subsurface flow and transport.

Together, the three SFA Challenges explore linkages between fundamental processes and overall system responses from the **molecular to the field-scales**.

ORGANIZATION & APPROACH

Sustainable Systems SFA
Tackling Three Key Challenges that Hinder Predictive Understanding of Flow and Transport Through Complex Subsurface Systems by Considering the Nature and Interaction of Fundamental Mechanisms as well as their Macroscopic Manifestations
LRM, Susan Hubbard
Project Business Manager, Lisa Kelly

Modeling Lead, Carl Steefel

Challenge: Unraveling Biogeochemical Pathways
Lead, Harry Beller

Focus: Quantification of interrelated microbial metabolic and geochemical mechanisms

Site: Hanford 100H

LBNL Scientific Staff: Markus Bill, Eoin Brodie, Shaun Brown, John Christensen, Mark Conrad, Boris Faybishenko, Jil Geller, Peter Nico, Eric Sonnenthal, Carl Steefel, Li Yang

LBNL Postdocs: Ruyang Han, Ulas Karaoz, Liping Qin, Sergi Molins Rafa, Charuleka Varadharajan, Chris Wanner

Collaborators: Adam Arkin (LBNL, UCB), Jim Fredrickson (PNNL), Yohisko Fujita (INL), Allan Konopka (PNNL), and Scott Peterson (CH2M Hill)

Challenge: Evolution of Pore Structures and Flowpaths
Lead, Ken Williams

Focus: Quantification of feedbacks between biogeochemical transformations and flow characteristics

Site: Rifle (IFRC)

LBNL Scientific Staff: Eoin Brodie, Jonathan Ajo-Franklin, Jinsong Chen, Mark Conrad, Don DePaolo, Hoi-Ying Holman, Susan Hubbard, Mike Kowalsky, Peter Nico, Dimitris Silin, Carl Steefel, Tetsu Tokunaga, Yuxin Wu, Li Yang

LBNL Postdocs: Baptiste Dafflon, Sergi Molins Rafa

Collaborators: John Barger (SLAC), Li Li (Penn State), Phil Long (LBNL), Bill Moses (LBNL), and the Rifle IFRC Team

Challenge: Predicting Contaminant Mobility at the Plume Scale
Lead, Jim Davis

Focus: Development of approaches for integrating geochemical mechanisms with hydrogeological heterogeneity for tractable plume-scale predictions

Site: Savannah F-Area

LBNL Scientific Staff: Jinsong Chen, John Christensen, Wen Ming Dong, Patricia Fox, Susan Hubbard, Peter Nico, Nic Spycher, Will Stringfellow, Jiamin Wan

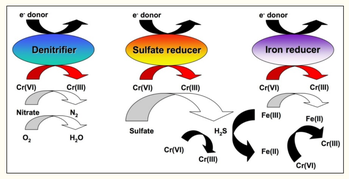
LBNL Postdocs: Sergio Bea, Haruko Murakami

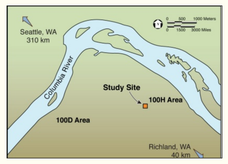
Collaborators: Miles Denham (SRNL), Jack Istok (OSU), Jim Hunt (UCB), Dan Kaplan (SRNL), John Seaman (SRNL), and the ASCEM team

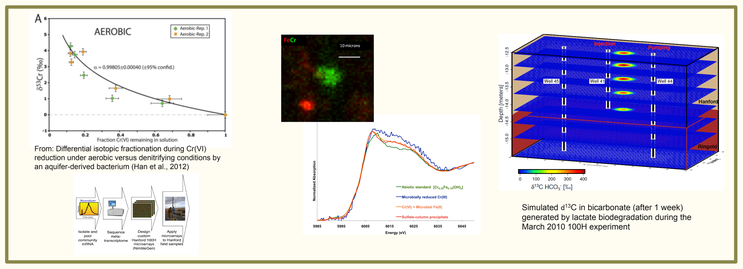
LOOKING FORWARD:
Sustainable Systems SFA Retreat, January 2011
Identifying Biogeochemical Grand Challenges relevant to a variety of DOE Mission Drivers

UNRAVELING BIOGEOCHEMICAL PATHWAYS CHALLENGE

- Focuses on quantification of critical and interrelated **microbial metabolic and geochemical mechanisms** associated with chromium in situ reductive immobilization and reoxidation
- Also developing **tools and approaches** that can be used to "unravel" complex biogeochemical reaction networks and help **bridge molecular to continuum scales**
- Tested at the Cr(VI)-contaminated **Hanford 100H Site**







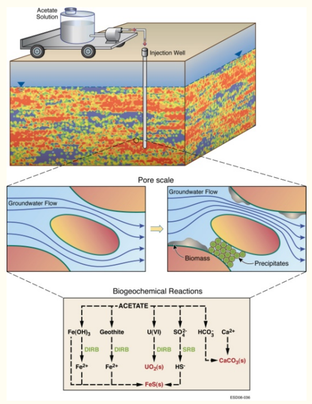
PLEASE VISIT POSTERS:
- Competing evidence for enzymatic vs. abiotic reduction of Cr(VI) in Hanford 100H flow-through columns (Varadharajan, Nico et al.)
- Use of metagenomic and meta-transcriptomic analysis to interpret biogeochemical processes mediated by Hanford 100H bacteria (Beller et al.)
- Reactive transport modeling of Hanford 100H lab- and field-scale experiments (Sonnenthal et al.)

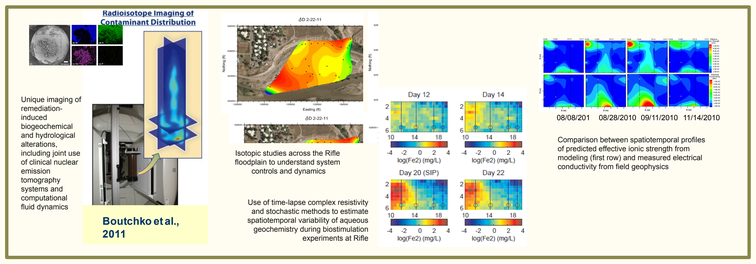
EVOLUTION OF PORE STRUCTURES AND FLOWPATHS CHALLENGE

Feedbacks between biogeochemical transformations and flow

- Quantification of reaction-induced dynamic porosity-permeability relationships in the subsurface,
- Assessment of their impact on elemental fluxes and contaminant mobility, and
- Identification of key variables and proxy signatures that are diagnostic of systems-level transitions and feedbacks.

The Evolution Challenge is conducted in close collaboration with Phil Long and the Rifle IFRC team



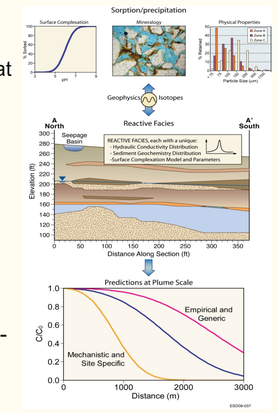


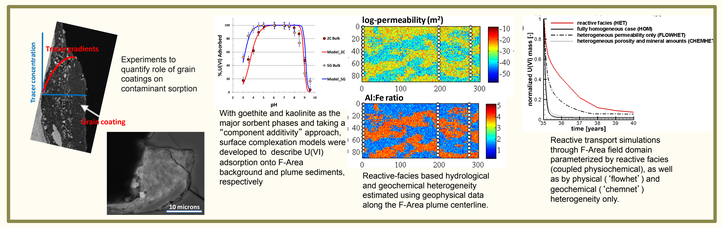
PLEASE VISIT POSTERS:
- Pore scale modeling of permeability evolution (Molins Raffa et al.)
- Isotopic signature of calcium and sulfur partitioning during biostimulation: experiments &simulations (Druhan et al)
- Highly depleted gypsum veins at the Rifle Site attributed to multiple episodes of redox cycling (Conrad et al)
- Field-scale estimation and simulation of biogeochemical heterogeneity (Chen et al.)

PREDICTING CONTAMINANT MOBILITY AT THE PLUME SCALE CHALLENGE

Investigating the integrated impact of coupled physiochemical heterogeneity on long term plume behavior

- Quantifying controls on contaminant behavior at the laboratory scale
- Developing and implementing a "reactive facies" concept to enable reliable predictive models of the fate and transport of contaminants at the plume scale and over site stewardship time frames.
- Exploring the necessary level of detail that is required for accurate simulations of long-term plume mobility.
- Conducted at the U-contaminated Savannah F-Area in close collaboration with Miles Denham the EM-sponsored AFRI and ASCEM projects.





PLEASE VISIT POSTERS:
- U(VI) mobility in acidic waste plumes: Laboratory analysis and surface complexation modeling (Wan et all)
- Reactive Facies: An approach for parameterizing plume-scale reactive transport models using multi-type, multi-scale datasets (Wainwright et al.)
- Determining the plume source discharge, trailing edge, and natural attenuation timeframe: the F-area Savannah River Site (Tokunaga et al.(
- Integrating geochemical, reactive transport, and facies-based modeling approaches to assess U(VI) contamination at the Savannah F-Area (Bea et all)

FY12 PUBLICATIONS

Including SFA-led papers (**in bold**) and SFA-collaborative efforts

- **Armstrong, R., Ajo-Franklin**, J. "Investigating Biomineralization using Synchrotron based X-Ray Computed Microtomography." Geophysical Research Letters, 38, L08406, 4 PP., 2011.
- Barkouki, T.H., Martinez, B.C., Mortensen, B.M., Weathers, T.S., De Jong, J.D., Ginn, T.R., Spycher, N.F., Smith,R.W., Fuijita, Y., Forward and inverse bio-geochemical modeling of microbially induced calcite precipitation in half-meter column experiments, Springer, Vol. 90, Number 1, 23-39, 2011.
- **Berryman,** J., "Bounds and self-consistent estimates for elastic constants of granular polycrystals composed of orthorhombics or crystals with higher symmetries. Physical Review E, 83, 046130, 2011.
- **Boutchko**, R., Rayz, V., Vandehey, N., O'Neil, J., Budinger, T., Nico, P., Druhan, J., Saloner, D., Gullberg, G., Moses, W., Imaging and modeling of flow in porous media using clinical nuclear emission tomography systems and computational fluid dynamics, Journal of Applied Geophysics, Vol 76, PP 74-81, 2011.
- **Brodie,** E. L., D. C. Joyner, B. Faybishenko, M. E. Conrad, C. Rios-Velazquez, B. Mork, R. Kelley, A. Willet, S. Koenigsberg, D. Herman, M. K. Firestone, and T. C. Hazen, Evaluation of sustained release polylactate electron donors for removal of hexavalent chromium from contaminated groundwater. Chemosphere, 85:660-665, 2011.
- **Commer,** M., Newman, G. A., Williams, K. H., and Hubbard, S. S. "Three-dimensional induced polarization data inversion for complex resistivity." Geophysics, Vol. 76, No. 3, P. F157-171, 2011.
- **Finsterle, S**., and Kowalsky, M.B., A truncated Levenberg-Marquardt algorithm for the calibration of highly parameterized nonlinear models, Computers and Geosciences, 37(6), 731-738, 2011.
- **Flores Orozco,** A., K.H. Williams, P.E. Long, S.S. Hubbard and A. Kemna, Using spectral induced polarization (SIP) to infer biogeochemical processes associated with bioremediation of a uranium-contaminated aquifer, JGR-Biogeosc, 116, G03001, 2011.
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- **Li, L.,** Gawande, N., Kowalsky, M.B., Steefel, C., Hubbard, S., Physicochemical heterogeneity controls on uranium bioreduction rates at the field scale. Environmental Science and Technology, 45 (23): 9959-9966 2011.
- Mohanty, S. R., B. Kollah, E. L. Brodie, T. C. Hazen, and E. E. Roden. 2011. 16S rRNA Gene Microarray Analysis of Microbial Communities in Ethanol-Stimulated Subsurface Sediment. Microbes and Environments doi:10.1264/jsme.ME11111.
- Scheibe, T., S. Hubbard, T.C. Onstott and M.F. DeFlaun, Lessons Learned from Bacterial Transport Research at the South Oyster Field Research Site, Ground water, Vol. 49, Issue 5, pages 745-763, 2011.
- **Wan, J**., Dong, W. and Tokunaga, T., "Method to Attenuate U(VI) Mobility in Acidic Waste Plumes Using Humic Acids," Environmental Science & Technology, 2011. composition: Proteogenomic analysis of the citrate synthase protein during bioremediation of U(VI). Microbial Biotechnology, 4 (1), 55–63, 2011.
- Wilkins, M.J., S.J. Callister, M. Miletto, K.H. Williams, C.D. Nicora, D.R. Lovley, P.E. Long, and M.S. Lipton: Development of a biomarker for Geobacter activity and strain composition: Proteogenomic analysis of the citrate synthase protein during bioremediation of U(VI). Microbial Biotechnology, 2011.
- Williams, K. H., P. E. Long, J. A. Davis, C. I. Steefel, M. J. Wilkins, A. L. N'Guessan, L. Yang, D. Newcomer, F. A. Spane, L. J. Kerkhof, L. McGuinness, R. Dayvault, and D. R. Lovely, Acetate availability and its influence on sustainable bioremediation of uranium-contaminated groundwater. Geomicrobiology Journal, 28(5-6 SP ISS) 519-539, 2011.
- **Wu, Yuxin**, Ajo-Franklin, J., Spycher, N., Hubbard, S., Zhang, G., Williams, K., Taylor, J., Fujita, Y., Smith, R., Geophysical monitoring and reactive transport modeling of ureolytically-driven calcium carbonate precipitation. Geochemical Transactions-Chemistry Central, doi:10.1186/1467-4866-12-7, 2011.
- **Dong, W.**, Tokunaga, T., Davis, J, Wan, J., Uranium(VI) adsorption and surface complexation modeling onto background sediments from the F-Area Savannah River Site, Environmental Science and Technology, 46, 1665-1571, 2012.
- **Han, R**., Qin, L.,Brown, S.T., Christensen, J.N., Beller, H.R., Differential isotopic fractionation during Cr(VI) reduction under aerobic verus denitrifying conditions by an aquifer-derived bacterium, Applied and Envi. I Microbiology, 78(7) 2462-4, 2012.
- **Wan, J.,** Tokunaga, T., Dong, W., Denham, M., Hubbard, S.S., Persistent source influences on the trailing edge of a groundwater plume, and natural attenuation timeframes: The F-Area Savannah River Site, Environmental Science and Technology, 2012 web released, dx.doi.org/10.1021/es204265q.

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