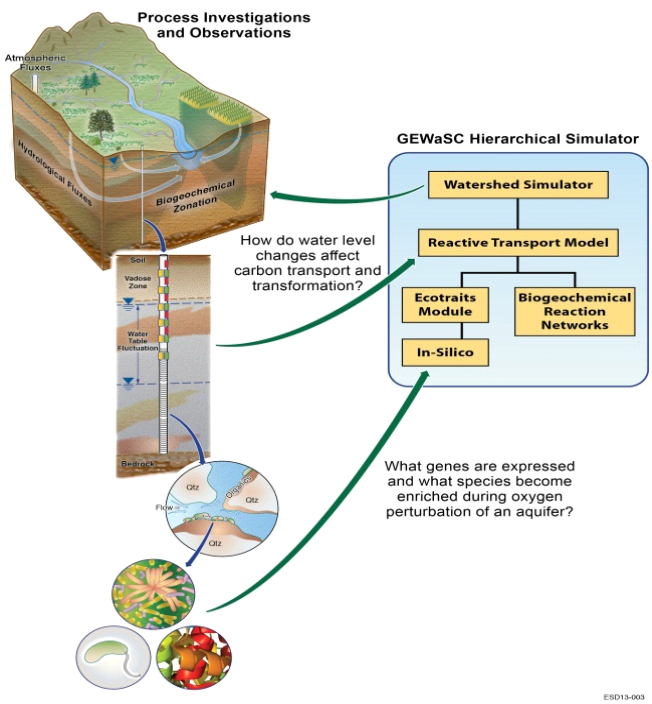
Sustainable Scientific Focus Area Systems

GENOMES TO WATERSHEDS

E-Newsletter for the LBNL Sustainable Systems Scientific Focus Area (SFA)

Issue 1 / Volume 1 / Spring 2014



Pioneering a Predictive Understanding of Genome-Through-Watershed-Scale Interactions and Feedbacks To Enable New Environmental and Energy Solutions
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Welcome to the first issue of the Sustainable Systems Scientific Focus Area (SFA) 2.0 quarterly e-newsletter. These e-newsletters will communicate our latest progress in understanding and predicting the complex interactions among microbes, minerals, and fluids in complex terrestrial environments.

Susan S. Hubbard SFA Lead

Introduction: Sustainable Systems 2.0:

Earth's terrestrial environment is enormously complex: it is the host for a multitude of interactions among plants, animals, microorganisms, minerals, migrating fluids, and dissolved constituent. These interactions occur within a heterogeneous framework across a wide range of scales. Because belowground terrestrial processes are perhaps the least understood component of terrestrial systems, processes occurring in this domain lead to significant uncertainties for the predictive understanding of biogeochemical cycling and system functioning relevant to carbon cycling, contaminant mobility, and biofuel crop sustainability. The Sustainable Systems SFA 2.0 is a new team-based DOE project that focuses on advancing approaches for quantifying and simulating genome-through-watershed scale interactions that govern biogeochemical cycling in these complex terrestrial environments.

Grand Challenge: Quantify how climate or land-use-induced changes in hydrology and vegetation affect subsurface carbon inputs, spatial and temporal distribution of flow, biogeochemical cycling, and microbial metabolic activity. Quantify how these processes change over time and what effect these interactions have on overall watershed biogeochemical functioning.

Grand Deliverable: Development of a Genome-Enabled biogeochemical Watershed Simulation Capability (GEWaSC) for quantifying how genomic information stored in a subsurface microbiome affects biogeochemical watershed functioning, how watershed-scale processes affect microbial functioning, and how these interactions co-evolve.

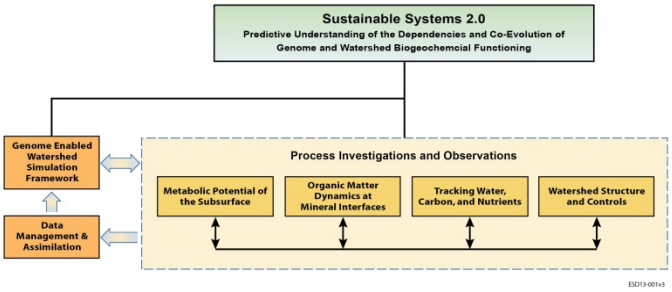
ABOUT OUR FIELD SITE—Rifle, CO:

The primary field site for the early stages of the SFA 2.0 research is a floodplain on the Colorado River located near the town of Rifle, CO.

The Rifle floodplain provides a wealth of existing data for this study, as well as an excellent test bed to interrogate how global change affects biogeochemical systems functioning. As a semi-arid region within the Upper Colorado River Basin, the Rifle area is threatened by various manifestations of climate change (including drought, diminished snowpack and earlier snowmelt, wildfires, and pest outbreaks), all of which have largely unexplored impacts on ecosystem services provided by the Colorado River corridor and its floodplain. Seasonal snowmelt leads to a natural hydrological pulse to the Rifle floodplain system, offering a natural perturbation to study hydrological-driven biogeochemical responses.

At this site, we are conducting the first coordinated attempt to quantify the metabolic potential of an entire subsurface ecosystem, which requires an understanding of the underlying genetic, biochemical, and physiological basis of microbial activity in the context of floodplain-wide fluxes and biogeochemical processes that occur within a heterogeneous aquifer.

The Rifle site management and infrastructure also supports and encourages scientific involvement by both national laboratory and university investigators at the site. The site plays an important role as community subsurface biogeochemistry testbed, where SFA scientists and "friends of Rifle" can develop critical understanding and capabilities, with a new focus on predicting metabolic and geochemical responses to climate-induced environmental perturbations. Read more about The Rifle site…



ABOUT OUR STRUCTURE:

The SFA 2.0 is composed of six key components: (1) Metabolic Potential; (2) Organic Matter Dynamics at Mineral Interfaces; (3) Tracking Water Carbon and other Nutrients; (4) Watershed Controls, (5) Data Management and Assimilation; and (5) Genome Enabled Watershed Simulation Capability (GEWaSC). Cross-component research coordination is centered around laboratory and field perturbation experiments, as required for developing GEWaSC and addressing the associated scientific challenges. SFA 2.0 is multi-institutional and multidisciplinary, with a total of ~60 technical staff working on the project.

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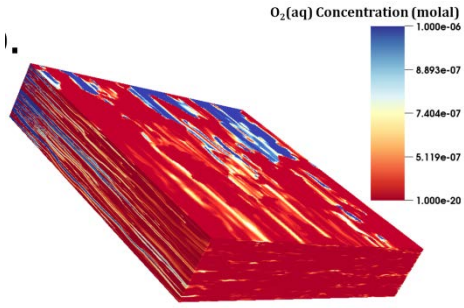
COMPONENT OVERVIEWS & RESEARCH UPDATES:

The ***Genome Enabled Watershed Simulation Capability (GEWaSC)*** *is a simulation framework for exploring interactions and feedbacks between microbial metabolic potential/activity, hydrology, and watershed biogeochemistry.*
Leads: Carl Steefel and Eoin Brodie

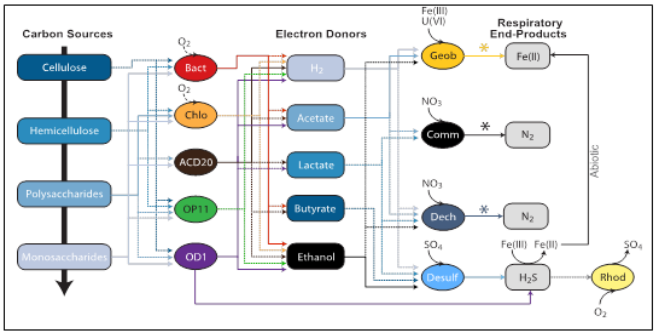
Preliminary work focuses on carbon and nitrogen cycling at the Rifle Flood Plain site and is being carried out at four scales: (1) development of microbial trait-based (EcoTrait) simulation capabilities based on genomic studies and designed for integration with flow and transport models; (2) 1-D and 2-D simulations along a transect through the Rifle Flood Plain, using both vadose-zone and groundwater properties and processes; (3) 3-D simulations of the Rifle Floodplain focusing on seasonal oxygen consumption and Naturally Reduced Zones (NRZ). This effort requires an initial simulation of the flood-plain-scale flow rates and aquifer thickness , and 4) simulations of the greater Rifle watershed, with a focus on the contribution of upland subsurface groundwater fluxes and the role of heterogeneities in establishing the sub-oxic status of the aquifer (see figure below). One key focus is on the effects of both seasonal and longer-term climactic and land-use changes on the biogeochemical and microbial function in an alluvial flood plain aquifer that contributes to the Colorado River system.



Simulation of oxygen concentrations in the Rifle Flood Plain using the ParCrunch parallel simulator. (simulations by Joe Beisman, Colorado School of Mines).

The ***Metabolic Potential (MP)*** *of the subsurface component is quantifying prevalent metabolic pathways in subsurface microbial communities that mediate carbon and electron flux.*
Leads: Harry Beller and Jill Banfield

A significant investment is being made in genome recovery for microorganisms in aquifer sediment and groundwater, as well as for those that respond to experimental and natural perturbations of the Rifle, CO field site environment (e.g., by addition of oxygen or nitrate). To date, we have acquired around 2.5 Tbp of DNA sequence information, as well as some linked transcriptomic and proteomic datasets. Using newly developed bioinformatics methods, we have reconstructed well over 1,000 draft genome sequences, almost all for organisms that are novel at the genus or higher level. Hundreds of genomes derive from organisms affiliated with bacterial and archaeal phyla that have no cultivated representatives. Thus, our analyses are providing the first insight into the metabolic roles of these organisms in biogeochemical cycles. We have also observed the emergence of known S- and Fe(II)-oxidizing chemolithoautotrophic bacteria in groundwater microbial communities under certain conditions, as supported by phylogenetic and proteomic data. Proteomic and transcriptomic data will allow us to probe the activity of specific pathways and, where possible, well-controlled laboratory experiments with aquifer sediments and bacterial isolates will provide information about metabolism of native carbon and responses to perturbations (such as oxygen or nitrate amendment) to compare with field results. In combination, the genome features, predicted metabolic capacities, experimental studies and evidence for function *in situ* are key inputs to the GEWaSC simulation effort.

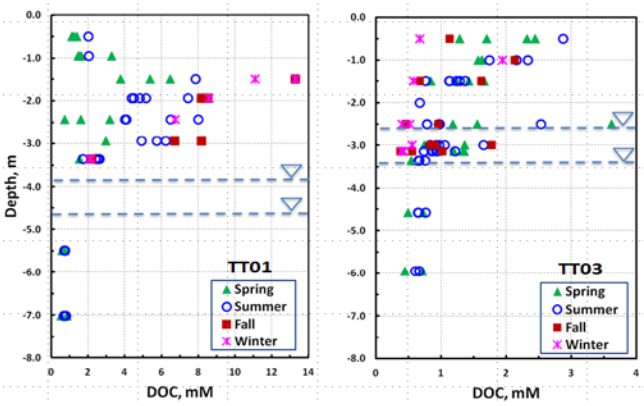


Wrighton et al. (2014) ISME J., doi: 10.1038/ismej.2013.249

*The **Tracking** component focuses on quantifying inventories and fluxes of C, N, and water in and across key subsurface compartments.*
Lead: Tetsu Tokunaga

Understanding these fluxes within the vadose zone and groundwater of semi-arid regions is challenging because of low soil organic carbon (SOC) inventories, low dissolved organic carbon (DOC) fluxes, and slow changes in soil inorganic carbon (SIC) inventories.

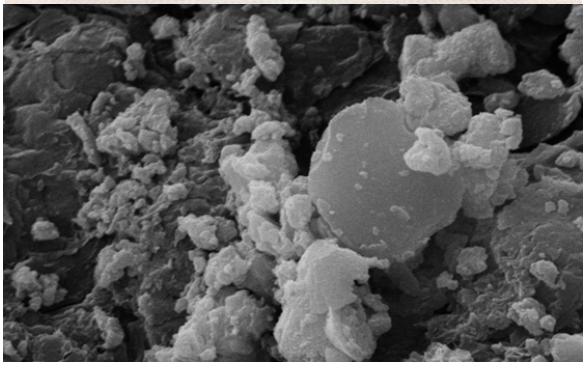
Within the Rifle floodplain, we recently installed monitoring and sampling instruments along a transect aligned with the groundwater flow direction, to determine seasonal infiltration, evapotranspiration, capillary fringe-groundwater interactions, and inventories and fluxes of water, carbon, and other components. Our recent sampling and analyses have revealed surprisingly high concentrations of DOC (>10 mM) in the vadose zone (see figure below), which seasonally contribute DOC to groundwater. In addition, mobile particulate organic carbon (POC) has been collected in the capillary fringe. This information is being combined with other analyses (hydraulic properties, geochemistry, isotope geochemistry, temperature profiles) to quantitatively understand fluxes of water, DIC, DOC, POC, and nutrients from the vadose zone into groundwater.



Dissolved organic carbon concentrations (DOC) in the vadose zone and groundwater in two wells at the Rifle Site.

*The **Organic Matter Dynamics (OMD)** at Mineral Interfaces component is determining mechanisms by which organic-mineral associations affect subsurface C and electron fluxes.*
Lead: Peter Nico

The component is working to provide chemical structure information on organic matter associated with sediment in the saturated zone. A comparison of Fourier transform infrared (FTIR) spectroscopy data collected on samples provided by the watershed controls component shows increased aromatic carbon in high organic matter hotspots across the site, consistent with the observed higher content of particulate plant-derived material. Furthermore, FTIR analysis of sediment incubations conducted by the metabolic potential component shows a noticeable decrease in aromatic associated functionality after incubations of sediments from those high organic matter hotspots.

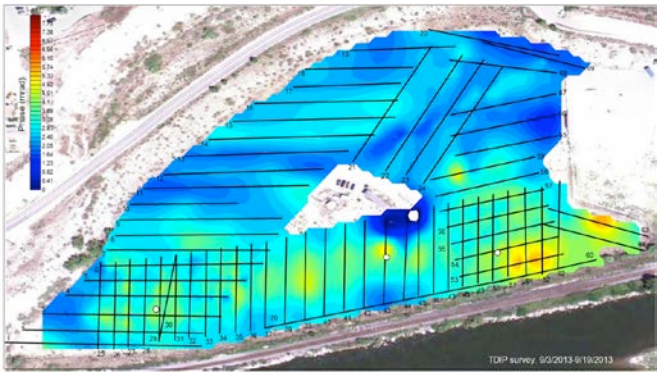


Photograph of sediment from Rifle, CO. site being examined for the release of organic matter (Top Figure).

SEM image of organic matter co-precipitated with iron mineral formed during a field experiment at the Rifle Co site. Scale = ~5 microns tall by ~8.5 microns wide (Bottom Figure)

The goal of the ***Watershed Controls*** *component is the development of a scale-dependent, yet integrated understanding of the primary factors controlling hydrobiogeochemical processes and nutrient cycling at the watershed scale.*
Lead: Kenneth H. Williams

An initial focus of the Watershed Controls component of the SFA is to use geophysical methods to identify regions of the Rifle, CO, subsurface that may serve as "hotspots" for a diverse range of microbial activity. Working with collaborators Dr. Adrián Flores Orozco (Technical University of Vienna) and his student Matthias Bücker (University of Bonn), SFA 2.0 scientists conducted a floodplain-wide induced polarization (IP) survey to characterize the distribution of organic matter and minerals (see figure below). Deposited during overbank deposition, the localized accumulation of organic matter and reduced, reactive mineral phases enables a wide variety of heterotrophic and lithotrophic microbial activity. Such accumulations thus constitute microbial "hotspots" in comparison to regions of the aquifer not enriched in such materials; SFA research is exploring the role that they play in the overall biogeochemical functioning of the floodplain.

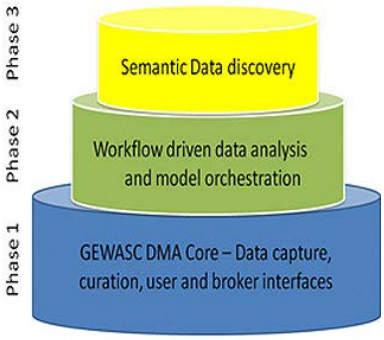


Geophysical characterization of hotspots distributed throughout the Rifle floodplain

The ***Data Management and Assimilation*** *(DMA) component is an agile data ecosystem to enable investigations and simulations of genome-to-watershed-scale processes.*
Lead: Deb Agarwal

The DMA component is developing a cyber-infrastructure to allow researchers to efficiently manage, find, and use data. The long-term structure of the effort is shown in the figure below.

There are three areas in which effort is currently concentrated: (1) the Rifle data management system, which has been upgraded to include a variety of new datasets—the user interface and plotting capabilities have also been upgraded to provide additional multi-well plotting capabilities; (2) the development of use cases that will provide guidelines for data fusion across data sources—one use case under development combines ggkbase and Rifle data to allow microbe abundance and function to be integrated with other measurements; and (3) the geochemical datasets, including laboratory experimental results and field wellbore measurements.



Development phases for SFA 2.0 cyber-infrastructure, culminating in advanced data analysis and data discovery capabilities.

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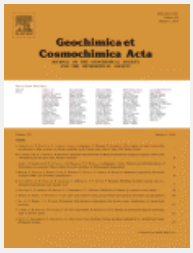
FEATURED PUBLICATIONS:

SFA 2.0 members publish in a variety of high impact journals. A few recent highlights are provided below; please visit our website to see a full list of our publications

A recent article entitled "Small genomes and sparse metabolisms of sediment – associated bacteria from four candidate phyla." (Kantor et al., 2013) was honored by the journal *mBio* as an "Editor's Pick" for the journal's October-November 2013 issue. *mBio* is published by the American Society for Microbiology. Read more about several related SFA 2.0 advances in understanding the terrestrial environment metabolic potential from the Banfield Lab.

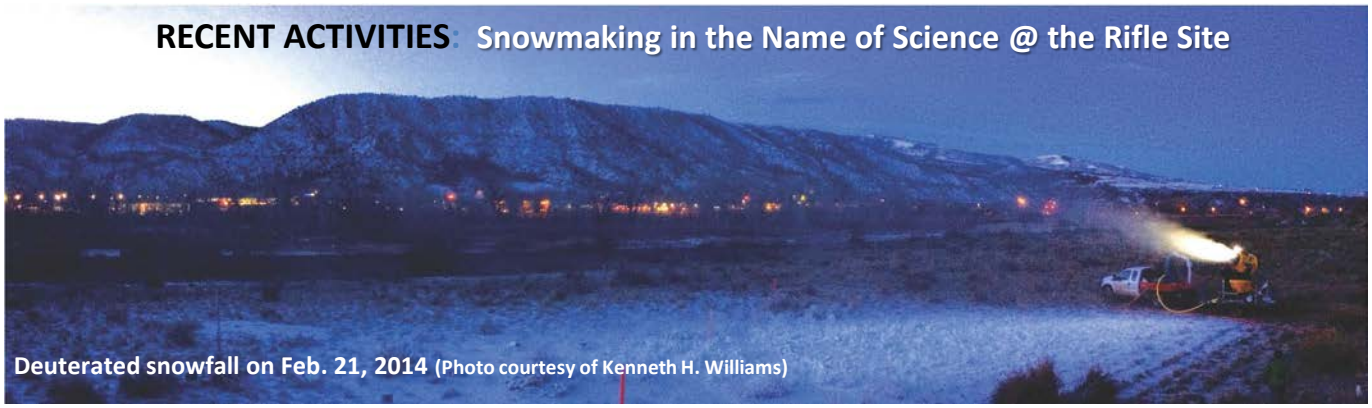
A paper entitled "Data-driven approach to identify field-scale biogeochemical transitions using geochemical and geophysical data and hidden Markov models: Development and application at a uranium contaminated aquifer," by Jinsong Chen, Susan Hubbard, and Ken Williams was published in Water Resources Research. This study develops a data-driven, statistical model to identify biogeochemical transitions using various time-lapse aqueous geochemical measurements and induced polarization (IP) data. The study results show that when considered together, aqueous geochemical data and IP imaginary conductivity provide diagnostic signatures of redox stages. This implies that the use of geophysical data could advance the possibility of using non-invasive methods to monitor critical biogeochemical- system stages and transitions remotely and over field- relevant scales. Read more



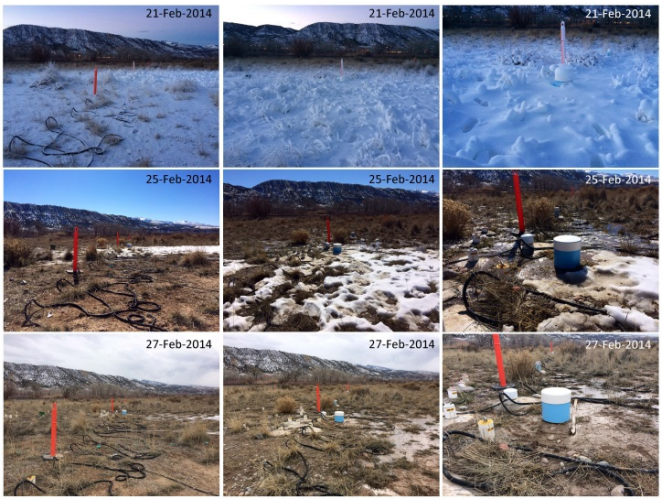
A recent paper entitled "Calcium isotope fractionation in groundwater: Molecular scale processes influencing field scale behavior," by Jennifer Druhan, Carl Steefel, Ken Williams, and Don DePaolo, was published in *Geochimica et Cosmochimica Acta*. The study reports on the development of an isotope-specific model for calcite precipitation that can be used to quantify the net fractionation in δ^{44}Ca associated with mineral growth during a transient or "'free drift"' departure from equilibrium. This treatment extends steady- state models for metal- isotope fractionation to transient systems and further demonstrates incorporation of an ion-by-ion growth model to reproduce observed trends where necessitated by fluid chemical composition. The model is applied to reproduce observed calcium concentration and δ^{44}Ca trends measured in clogged well bores at the Rifle, Colorado bioremediation field site. Read more

A paper entitled " Genome-enabled studies of anaerobic, nitrate-dependent iron oxidation in the chemolithoautotrophic bacterium *Thiobacillus denitrificans*," by Harry Beller and co-workers, was recently published in *Frontiers in Microbiology*. In this most extensive study to date on anaerobic, nitrate-dependent iron oxidation—which involved extensive whole-genome transcriptional studies, targeted gene knockouts, and random transposon-generated gene knockouts—the relationship between nitrate-dependent iron and uranium oxidation was explored, as well as the role of *c*-type cytochromes in these processes. The results have implications not only for the long-term efficacy of *in situ* reductive immobilization of uranium in contaminated aquifers, but also for our understanding of the fundamental process of reverse electron transfer in chemolithotrophic bacteria. Read more

RECENT ACTIVITIES: Snowmaking in the Name of Science @ the Rifle Site



Deuterated snowfall on Feb. 21, 2014 (Photo courtesy of Kenneth H. Williams)



A time series of photos tied to the deuterated snowfall and now snowmelt (Photos courtesy of Kenneth H. Williams).

SFA 2.0 scientists used snowmaking machines from the Aspen Ski Area to track infiltration of deuterium-labeled snow into soil, sub-soil sediments, and eventually into groundwater at the Rifle site. At Rifle, low oxygen, low nitrate conditions are typical in groundwater, except during water table rise or vertical water flux. During these times, nitrogen cycling increases nitrate concentration, which in turn oxidizes reduced metals and influences organic carbon flux and stability. Through intensive biogeochemical characterization coordinated with the labeled snowmelt infiltration, this experiment will allow us to understand and accurately predict subsurface biogeochemical functioning under a wide range of moisture conditions.

Light UAVs (unmanned Ariel Vehicles) for Terrestrial Research

Photo courtesy of John Peterson

With the importance of jointly monitoring above- and belowground processes at the Rifle site, SFA 2.0 investigators will jointly acquire and invert time lapse, surface-based geophysical data, together with datasets collected above the ground surface. The Earth Science Division at LBNL is currently pursuing approval from the FAA to perform UAV monitoring at Rifle and other sites.

SFA 2.0 EARLY CAREER SPOTLIGHT: BHAVNA ARORA

Bhavna Arora has been a postdoctoral Fellow at the Berkeley Lab's Earth Sciences Division since 2012. She received her Ph.D. from the interdisciplinary Water Management and Hydrological Science program at Texas A&M University, where she studied the effect of subsurface heterogeneity on modeling coupled biogeochemical processes in variably saturated porous media. Apart from reactive transport modeling, her recent research is aimed at multidisciplinary assessments of biogeochemical variables in landfill and waste-management sites. At these sites, the release of contaminants is controlled by multiple geochemical, hydrological, and microbiological factors, and occurs across various time scales. Since these controlling biogeochemical factors are nonlinear and complex, changes to measured water chemistry parameters can indicate the influence of multiple processes simultaneously. The answer lies in wavelet analysis, which can simultaneously point to the dominant patterns in the data and help in unraveling some of the inter-linkages. In this context, Bhavna has applied wavelet analysis to the Rifle site data. Wavelet analysis there revealed a 4-month periodicity in conservative solutes like sulfate and chloride from the anthropogenically contaminated zone. This work is providing strong evidence of coupled hydrologic-biogeochemical interactions dominating biogeochemical processes at the Rifle site. Bhavna will present this research at the 2014 TES/SBR Joint PI Meeting in Washington, DC May 6-7, 2014.

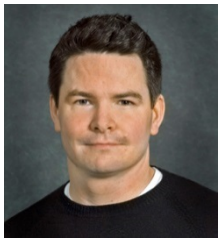
On a personal note: When Bhavna is not busy working on her passion for research, she enjoys traveling. Also, as is the case with most Earth scientists, she enjoys spending time in the great outdoors biking, hiking, and more recently kayaking. She also has a love of cooking and writing poems.

AWARDS and ACHIEVEMENTS:

Baptiste Dafflon received the 2013 Paul Niggli Medal, Switzerland's most prestigious "young scientist award" in the earth sciences

Susan Hubbard was honored as a '2013 Outstanding Women @ the Lab'

Jenny Druhan won the Best Junior Scientist Presentation award at the EnvironMetal 2013



Eoin Brodie awarded the Royal Netherlands Academy of Arts and Sciences, Visiting Professorship 2014.

SFA 2.0 Members presenting at many UPCOMING EVENTS:

May 6-7, 2014

TES/SBR Joint PI Meeting

SFA 2.0 Team members will participate in this annual PI meeting held in the DC area, including plenary presentations by Carl Steefel/Eoin Brodie on GEWaSC, and by Jill Banfield on Metabolic Potential. In addition, several researchers will present posters.

June 6-14, 2014

Seventeen SFA 2.0 presentations will be delivered at the June Goldschmidt conference, including a few keynotes and invited presentations:

- Jill Banfield on "Prediction of the Biogeochemical Roles of Uncultivated Bacteria and Archaea in the Subsurface,"
- Ken Williams on "A Floodplain Perspective on Elemental Cycling and Uranium Plume Persistence
- Carl Steefel on "The GEWaSC Framework: Multiscale Modeling of Coupled Biogeochemical, Microbiological, and Hydrological Processes," and
- Cristina Cismasu's oral presentation on "Iron and Carbon Dynamics during the Reductive Transformation of Organic Matter-Rich Fe(III)

Other presenters include: Bhavna Arora, John Bargar, Wenming Dong, Boris Faybishenko, Patricia Fox, Susan Hubbard, Sergi Molins, Tetsu Tokunaga, Jiamin Wan, Ken Williams, and co-authors

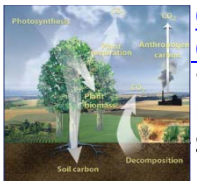
View full list of SFA 2.0 presentations here

July 6-11, 2014

GORDON RESEARCH CONFERENCE
Bates College, Lewiston, ME

Carl Steefel will present a talk entitled "Bridging the Gap from Pore to Continuum Scales in Reactive Transport" during the **Modeling Reactive Transport in Large-Scale Systems** session.

September 3-5, 2014



COMPLEX SOILS SYSTEMS CONFERENCE
"A Path to Improved Understanding of Complex Soils Systems"

Supported by SSSA/Bouyoucos Funds, Berkeley Lab, and DOE

Contributions are solicited from microbiologists, ecologists, biogeochemists, soil physicists, agricultural scientists, hydrologists, geophysicists, climatologists, and others working on key aspects of complex soil systems.

SFA 2.0 KEY COLLABORATORS:

The SFA 2.0 is sponsored by the U.S. Department of Energy, Biological, and Environmental Research, Subsurface Biogeochemical Research Program. David Lesmes, Program Manager, can be reached at David.Lesmes@science.doe.gov

QUESTIONS/COMMENTS:

Send any comments or questions concerning this newsletter to:

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