Sustainable Systems SFA 2.0

Participation in the December 15-19, 2014 American Geophysical Union (AGU) Meeting in San Francisco, CA

Funded by the United States Department of Energy, Office of Science, Biological and Environmental Research

Fall AGU sessions and presentations led by SFA 2.0 team members and key collaborators

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DOE Office of Science.

SFA- Chaired Sessions

B12A: Contaminant Biogeochemical Cycles and Elemental Speciation: Implications for Remediation of Subsurface Environments I

Session ID#: 3060

Monday, 15 December 2014: 10:20 AM-12:20 PM, *Moscone West 2004*

Chairs: Valerie K Stucker, GNS Science-Institute of Geological and Nuclear Sciences Ltd, Lower Hutt, New Zealand, **James F Ranville**, Colorado School of Mines, Golden, CO, United States and **Kenneth Hurst Williams**, Lawrence Berkeley National Laboratory, Earth Science Division, Berkeley, CA, United States

Primary Conveners: Valerie K Stucker, GNS Science, Marine Geosciences, Lower Hutt, New Zealand

Co-conveners: James F Ranville, Colorado School of Mines, Golden, CO, United States and **Kenneth Hurst Williams**, Lawrence Berkeley National Laboratory, Berkeley, CA, United States

B21B: Contaminant Biogeochemical Cycles and Elemental Speciation: Implications for Remediation of Subsurface Environments II Posters

Session ID#: 4699

Tuesday, 16 December 2014: 8:00 AM-12:20 PM, PM , *Moscone West Poster Hall*

Chairs: Valerie K Stucker, GNS Science-Institute of Geological and Nuclear Sciences Ltd, Lower Hutt, New Zealand, **James F Ranville**, Colorado School of Mines, Golden, CO, United States and **Kenneth Hurst Williams**, Lawrence Berkeley National Laboratory, Earth Science Division, Berkeley, CA, United States

Primary Conveners: Valerie K Stucker, GNS Science, Marine Geosciences, Lower Hutt, New Zealand

Co-conveners: James F Ranville, Colorado School of Mines, Golden, CO, United States and **Kenneth Hurst Williams**, Lawrence Berkeley National Laboratory, Berkeley, CA, United States

B31L: Soil Organic Matter Dynamics: Novel Techniques, Big Data, and Functional Models III
Session ID#: 4464
Wednesday, 17 December 2014: 8:00 AM-10:00 AM, *Moscone West 2022-2024*

SFA- Chaired Sessions

Chairs: Peter S Nico, Lawrence Berkeley Laboratory, Berkeley, CA, United States, **Nancy J Hess**, Pacific Northwest National Laboratory, Environmental Molecular Sciences Laboratory, Richland, WA, United States and **Jinyun Tang**, Lawrence Berkeley Natl Lab, Berkeley, CA, United States
Primary Conveners: Lucas E Nave, University of Michigan, Ann Arbor, MI, United States
Co-conveners: Christopher Swanston, USDA Forest Service, Houghton, MI, United States, **Margaret S Torn**, Berkeley Lab/UC Berkeley, Berkeley, CA, United States and **Nancy J Hess**, Pacific Northwest National Laboratory, Environmental Molecular Sciences Laboratory, Richland, WA, United States

SFA- Chaired Sessions

B33B: Characterizing Spatial and Temporal Variability of Hydrological and Biogeochemical Processes Across Scales I Posters
Session ID#: 4696
Wednesday, 17 December 2014: 1:40 PM-6:00 PM , *Moscone West Poster Hall*

Chairs: Susan S. Hubbard, Lawrence Berkeley National Laboratory, Berkeley, CA, United States and **Bhavna Arora**, Lawrence Berkeley National Lab, Berkeley, CA, United States
Primary Conveners: Bhavna Arora, Lawrence Berkeley National Lab, Berkeley, CA, United States
Co-conveners: Haruko Murakami Wainwright, Lawrence Berkeley National Lab, Berkeley, CA, United States and **Susan S. Hubbard**, Lawrence Berkeley National Laboratory, Berkeley, CA, United States

B44B: Characterizing Spatial and Temporal Variability of Hydrological and Biogeochemical Processes Across Scales II
Session ID#: 2222
Thursday, 18 December 2014: 4:00 PM-6:00 PM, *Moscone West 2004*

Chairs: Haruko Murakami Wainwright[1], **Susan S. Hubbard**[1] and **Bhavna Arora**[2], (1)Lawrence Berkeley National Laboratory, Berkeley, CA, United States(2)Lawrence Berkeley National Lab, Berkeley, CA, United States
Primary Conveners: Bhavna Arora, Lawrence Berkeley National Lab, Berkeley, CA, United States
Co-conveners: Haruko Murakami Wainwright, Lawrence Berkeley National Lab, Berkeley, CA, United States and **Susan S. Hubbard**, Lawrence Berkeley National Laboratory, Berkeley, CA, United States

B11H-0153: Metatranscriptomic Analysis of Groundwater Reveals an Active Anammox Bacterial Population

Monday, December 15, 2014

08:00 AM - 12:20 PM, *Moscone West Poster Hall*

Talia N. M. Jewell[1], *Ulas Karaoz*[1], *Brian C Thomas*[2], *Jillian F Banfield*[2], *Eoin Brodie*[1], *Kenneth Hurst Williams*[1] *and Harry R Beller*[1], *(1)Lawrence Berkeley National Laboratory, Berkeley, CA, United States, (2)University of California Berkeley, Berkeley, CA, United States*

Abstract Groundwater is a major natural resource, yet little is known about the contribution of microbial anaerobic ammonium oxidation (anammox) activity to subsurface nitrogen cycling. During anammox, energy is generated as ammonium is oxidized under anaerobic conditions to dinitrogen gas, using nitrite as the final electron acceptor. This process is a global sink for fixed nitrogen. Only a narrow range of monophyletic bacteria within the Planctomycetes carries out anammox, and the full extent of their metabolism, and subsequent impact on nitrogen cycling and microbial community structure, is still unknown. Here, we employ a metatranscriptomic analysis on enriched mRNA to identify the abundance and activity of a population of anammox bacteria within an aquifer at Rifle, CO. Planktonic biomass was collected over a two-month period after injection of up to 1.5 mM nitrate. Illumina-generated sequences were mapped to a phylogenetically binned Rifle metagenome database.

We identified transcripts for genes with high protein sequence identities (81-98%) to those of anammox strain KSU-1 and to two of the five anammox bacteria genera, *Brocadia* and *Kuenenia*, suggesting an active, if not diverse, anammox population. Many of the most abundant anammox transcripts mapped to a single scaffold, indicative of a single dominant anammox species. Transcripts of the genes necessary for the anammox pathway were present, including an ammonium transporter (*amtB*), nitrite/formate transporter, nitrite reductase (*nirK*), and hydrazine oxidoreductase (*hzoB*). The form of nitrite reductase encoded by anammox is species-dependent, and we only identified *nirK*, with no evidence of anammox *nirS*. In addition to the anammox pathway we saw evidence of the anammox bacterial dissimilatory nitrate reduction to ammonium pathway (*narH*, putative *nrfA,* and *nrfB*), which provides an alternate means of generating substrates for anammox from nitrate, rather than relying on an external pool. Transcripts for hydroxylamine oxidoreductase (HAO) were abundant and more similar to known anammox HAO genes than those used in aerobic ammonia oxidation. The elevated levels of anammox transcripts suggest that anammox may play a significant role in nitrogen cycling within groundwater systems.

B21B-0039: Redox Fluctuation Influences Viral Abundance in the Reduced Zone of a Shallow Alluvial Aquifer in Rifle, CO

Tuesday, December 16, 2014

08:00 AM - 12:20 PM, *Moscone West Poster Hall*

Donald Pan[1], *Kenneth Hurst Williams*[2], *Mark Robbins*[2] *and Karrie A Weber*[1], *(1)University of Nebraska Lincoln, Lincoln, NE, United States, (2)Lawrence Berkeley National Laboratory, Berkeley, CA, United States*

Abstract Naturally reduced zones (NRZs) within alluvial aquifers contain naturally elevated concentrations of organic carbon (OC) and can play a role in controlling the fate of redox-active contaminants. OC in NRZs stimulates microbial activity through coupling of OC oxidation to reduction of subsurface electron acceptors. Stimulation of the indigenous microbial community also results in the stimulation of the viral community. Viruses are the most abundant biological entity on Earth and can indirectly influence carbon cycling by infecting and lysing host cells, resulting in release of OC bound in biomass. In the alluvial aquifer near Rifle, CO, prior acetate injection resulted in reductive immobilization of U and a reduced zone simulating a NRZ, with elevated ferrous iron and sulfide (53.2–62.5 µM and 0.2–3.1 µM, respectively). To study the effects of redox fluctuations in a RZ, oxygenated groundwater was injected. Prior to injection, groundwater was suboxic (0.05–0.11 mg/L). Amended O_2 was immediately consumed in the RZ. While cell numbers didn't significantly increase, viruses increased from $1.1x10^6$–$2.1x10^6$ mL^{-1} to $2.3x10^6$–$4.6x10^6$ mL^{-1}. VCR increased 1.8–3.4 fold from 3.9–10.1 to 11.0–17.9, demonstrating microbial activity. These changes were associated with large fluctuations of groundwater dissolved OC, suggesting viral release of OC from cellular biomass. Groundwater ORP decreased from an initial -146 mV – -132 mV to -317 mV – -304 mV, indicating an increase in the supply of available electron donors. Thus, rather than expected oxidative solubilization of U following amendment of O_2, soluble U decreased, suggesting likely U reduction in the RZ. Fe and S fluctuated, but changes were not associated with aqueous U. Across the whole floodplain, viral abundance is correlated to groundwater dissolved OC, suggesting that viruses may be contributing to the liberalization of dissolved OC from biomass in NRZs, allowing turnover of carbon and reduction of contaminants of interest, independent of external acetate amendment. This is especially important considering the role of OC in controlling the fate and transport of contaminants in aquifers. These results suggest that viruses are an important factor to consider in the turnover and retention of carbon in the subsurface.

B21B-0040: Importance of Organic Matter-Uranium Biogeochemistry to Uranium Plume Persistence in the Upper Colorado River Basin

Tuesday, December 16, 2014

08:00 AM - 12:20 PM, *Moscone West Poster Hall*

John Bargar[1], *Noemie Janot*[1], *Morris E Jones*[2], *Sharon E. Bone*[1], *Juan Lezama-Pacheco*[2], *Scott E Fendorf*[3], *Philip E Long*[4], *Kenneth Hurst Williams*[4] *and Richard P. Bush*[5], *(1)SLAC, Menlo Park, CA, United States, (2)Stanford University, Los Altos Hills, CA, United States, (3)Stanford University, Stanford, CA, United States, (4)Lawrence Berkeley National Laboratory, Berkeley, CA, United States, (5)DOE Office of Legacy Management, Office of Site Management, Grand Junction, CO, United States*

Abstract Recent evidence suggests that biologically driven redox reactions, fueled by sedimentary lenses enriched in detrital organic matter, play major roles in maintaining the persistent uranium groundwater plume in the subsurface at the U.S. Department of Energy's Rifle, CO field research site. Biogeochemical cycling of C, N, Fe, and S is highly active in these organic-rich naturally reduced zones (NRZs), and uranium is present as U(IV). The speciation of these elements profoundly influences the susceptibility of uranium to be reoxidized and remobiliized and contribute to plume persistence. However, uranim speciation in particular is poorly constrained in these sytems. To better evaluate the importance of NRZs to uranium mobility and plume persistence at the Rifle site, the DOE-BER-funded SLAC SFA team has characterized vertical concentration profiles and speciation of uranium, iron, sulfur, and NOM in well bores at high spatial resolution (4 inch intervals). Up to 95% of the sedimentary uranium pool was found to be concentrated in NRZs, where it occurs dominantly as non-crystalline forms of U(IV). Uranium accumulation and the presence of the short-lived sulfide mackinawite (FeS) at NRZ-aquifer interfaces indicate that NRZs actively exchange solutes with the surrounding aquifer. Moreover, sediment textures indicate that NRZs are likely to be abundant in riparian zones throughout the upper Colorado River basin (U.S.A.), which contains most of the contaminated DOE legacy uranium ore processing sites in the U.S. These results suggest that NRZ-uranium interactions may be important to plume persistence regionally and emphasize the importance of understanding molecular-scale processes.

B21B-0043: Clay Mineralogy of Soils and Sediments from an Alluvial Aquifer, Rifle, Colorado

Tuesday, December 16, 2014

08:00 AM - 12:20 PM, *Moscone West Poster Hall*

*Laura K Zaunbrecher[1], **W. Crawford Elliott**[1], David Lim[1,2], Rebecca A Pickering[1], Kenneth Hurst Williams[3], Philip E Long[4] and Nikolla P Qafoku[5], (1)Georgia State University, Atlanta, GA, United States, (2)University of Wisconsin Madison, Department of Geology and Geophysics, Madison, WI, United States, (3)Lawrence Berkeley National Laboratory, Berkeley, CA, United States, (4)Lawrence Berkeley National Lab, Chelan, WA, United States, (5)Pacific Northwest Natl Lab, Richland, WA, United States*

Abstract Alluvial aquifers along the Colorado River corridor in central to western Colorado contain legacy contamination including U, V, As and Se. These alluvial aquifers host important “hot spots” and “hot moments” for microbiological activity controlling organic carbon processing and fluxes in the subsurface that are both significant on their own, but also influence contaminant behavior. Mineral phases likely active in the sequestration of metal contaminants are chlorite, smectite-vermiculite, illite, and smectite. These minerals are also important biogeofacies markers. The Colorado alluvial sediments include lenses of silt and clay that are commonly more reduced than coarser grained materials. The clay minerals that make up the alluvial aquifer sediments include these mineral phases important for metal sequestration (chlorite, smectite, illite), as well as kaolinite and quartz. More specifically, the clay mineralogy of soils derived from these sediments at Rifle are composed of the same suite of minerals found in the alluvial sediments plus a vermiculite-smectite intergrade. The vermiculite-smectite intergrade is a weathering product of illite. The presence of illite and chlorite in both the sediments and the soils at Rifle reflect a mineralogically immature character of the source rocks. These assemblages are consistent with sediments and soils that formed in a moderately low rainfall climate, indicative of mixed provence of immature (chlorite, smectite, illite) and mature (kaolinite) minerals relative to their source areas.

B22D-08: Metatranscriptomic Evidence of Chemolithoautotrophy in the Rifle (CO) Subsurface Relevant to C, S, N, and Fe Cycling

Tuesday, December 16, 2014

12:05 PM - 12:20 PM, *Moscone West 2004*

Harry R Beller[1], *Talia N. M. Jewell*[1], *Ulas Karaoz*[1], *Brian C Thomas*[2], *Jillian F Banfield*[2], *Eoin Brodie*[1] *and Kenneth Hurst Williams*[1], *(1)Lawrence Berkeley National Laboratory, Berkeley, CA, United States, (2)University of California Berkeley, Berkeley, CA, United States*

Abstract Although there is a limited understanding of the chemolithoautotrophic activity of aquifer microorganisms, such subsurface microbial activity could greatly influence the cycling of elements such as C, S, N, and Fe. Here, we present transcriptional (RNA-Seq) evidence of the emergence of such chemolithoautotrophic activities in groundwater filter samples from a 2-month experiment in which up to 1.5 mM nitrate (a native electron acceptor) was injected into a perennially suboxic/anoxic aquifer (Rifle, CO) containing a large reservoir of reduced Fe- and S-containing compounds. Illumina sequence data from rRNA-subtracted cDNA libraries was assembled and mapped to phylogenetically binned Rifle metagenome data.
Indicative of the activity of Fe(II)-oxidizing bacteria, many high-abundance transcripts mapped to the Gallionellaceae family, whose known members are chemolithoautotrophic bacteria that catalyze Fe(II) oxidation. For example, included among the most abundant transcripts were a cold-shock protein and an acyl carrier protein with 96-98% protein sequence identity to *Gallionella capsiferriformans* and a nitrite reductase (*nirS*) gene likely belonging to a *Sideroxydans* relative. The apparent activity of Gallionellaceae members is consistent with 16S rRNA iTag analyses of these samples, which indicated that *Gallionella*-related taxa accounted for up to ~50% of these communities. Evidence of sulfide oxidation also was apparent in these samples. For example, highly expressed subunits of APS reductase were very similar to those of the obligately chemolithoautotrophic S- and Fe(II)-oxidizing *Thiobacillus denitrificans* in terms of sequence identity (98-99%) and synteny of the mapped scaffold. Also highly expressed were a ß-Proteobacterial Form II RubisCO gene and a hydrazine oxidoreductase gene (93% identity to the planctomycete KSU-1), the latter strongly indicative of anaerobic ammonia oxidation (anammox) activity, which has seldom been reported in aquifer environments. Such gene-level data on CO_2 fixation and Fe(II), sulfide, and ammonium oxidation in the Rifle subsurface will contribute to genome-enabled modeling efforts aimed at developing a predictive understanding of biogeochemical processes at the site as part of LBNL's Sustainable Systems Scientific Focus Area (SFA) 2.0.

B23B-0203: Seasonal variations and cycling of nitrous oxide using nitrogen isotopes and concentrations from an unsaturated zone of a floodplain

Tuesday, December 16, 2014

01:40 PM - 06:00 PM, *Moscone West Poster Hall*

Markus Bill[1], *Mark E Conrad*[1], *Sophie Kolding*[1], *Kenneth Hurst Williams*[1] *and Tetsu K Tokunaga*[2], *(1)Lawrence Berkeley National Laboratory, Berkeley, CA, United States, (2)Lawrence Berkely Natl Lab, Berkeley, CA, United States*

Abstract Nitrous oxide (N_2O) concentrations and isotope ratios of ^{15}N to ^{14}N of N_2O in the vadose zone mainly depend on atmospheric deposition, symbiotic or non-symbiotic N_2 fixation, and nitrification/denitrification processes in underlying groundwater. In an effort to quantify N_2O seasonal variations, cycling and N budgets in an alluvial aquifer in western Colorado (Rifle, CO), the concentrations and nitrogen stable isotopes of N_2O within the pore space of partially saturated sediments have been monitored over the 2013-2014 years. Vertically resolved profiles spanning from 0m to 3m depth were sampled at 0.5m increments at a periodicity of one month. At each of the profile locations, N_2O concentrations decreased from 3m depth to the surface. The maximum concentrations were observed at the interface between the unsaturated zone and groundwater, with minimum values observed in the near surface samples. The $d^{15}N$ values tend to increase from the unsaturated zone/groundwater interface to the surface. Both variation of N_2O concentrations and $d^{15}N$ values suggest that denitrification is the main contribution to N_2O production and both parameters exhibited a strong seasonal variation. The maximum concentrations (~10ppmv) were observed at the beginning of summer, during the annual maximum in water table elevation. The minimum N_2O concentrations were observed in the period from January to May and coincided with low water table elevations. Additionally, nitrogen concentrations and $d^{15}N$ values of the shallowest sediments within the vertical profiles do not show variation, suggesting that the main source of N_2O is associated with groundwater denitrification, with the shallower, partially saturated sediments acting as a sink for N_2O.

B31B-0016: Using Concentrations and Isotopic Compositions of CO_2 to Distinguish Microbial Production of CO_2in Unsaturated Zone Sediments in Hydrogeochemical Models

Wednesday, December 17, 2014

08:00 AM - 12:20 PM, *Moscone West, Poster Hall*

***Mark E Conrad**, Bhavna Arora, Kenneth Hurst Williams, Markus Bill, Nicolas Spycher, Carl I Steefel, Tetsu K Tokunaga and Susan S. Hubbard, Lawrence Berkeley National Laboratory, Berkeley, CA, United States*

Abstract Quantifying levels of microbial activity in unsaturated subsurface environments is an important factor for understanding exchange of greenhouse gases (e.g., CO_2, CH_4, N_2O) with the atmosphere. For CO_2, this is problematic due the variety of processes affecting its sources, fate and transport in the vadose zone (e.g., root respiration, carbonate dissolution and precipitation, exchange with pore water/groundwater and microbial production and consumption). To determine the impacts of all these processes and dependence on variables including temperature, moisture content and pH requires coupled numerical models supported by robust, long-term data sets. We are attempting to do this for a small (~90,000 m^2) floodplain adjacent to the Colorado River in the town of Rifle, Colorado. The geology of the site consists of 6-8 m of Quaternary alluvium composed of quartz and feldspar sands with silts, clays, pebbles, and cobbles overlying the less permeable Tertiary Wasatch Formation. The unsaturated zone is 3-4 m thick overlying a perched aquifer above the alluvium-Wasatch contact. Depth-distributed gas samplers and suction lysimeters for pore water sampling were installed at three locations across the site in March of 2013. From April 2013 to present, soil gas samples have been collected on a bi-weekly to monthly interval and analyzed for gas concentrations and isotopic compositions. Through the first year, several significant spatial and temporal trends have emerged from the data including higher soil gas CO_2 (up to 6% near the water table) with higher $\delta^{13}C$ values during the warmer summer months, possibly signifying higher levels of microbial activity. In the shallower soils, CO_2concentrations are lower (atmospheric to 2%) with more variable $\delta^{13}C$ values (ranging from -18‰ in the summer to -24‰ in the winter) likely due to slower exchange with the atmosphere during the winter when surface soils are more saturated due to snow cover and melting. Extensive data has also been collected on the concentrations and isotopic compositions of pore water organic carbon and groundwater DIC across the site in order to understand the effects of these components on carbon transport in the unsaturated zone. These data are being incorporated into a numerical model of the site that includes transport, chemical and biological reactions.

B31B-0019: Modeling the Biogeochemical Response of a Flood Plain Aquifer Impacted By Seasonal Temperature and Water Table Variations

Wednesday, December 17, 2014

08:00 AM - 12:20 PM, *Moscone West Poster Hall*

Bhavna Arora, *Nicolas Spycher, Sergi Molins and Carl I Steefel, Lawrence Berkeley National Laboratory, Berkeley, CA, United States*

Abstract With the overarching goal of understanding the impacts of climate and land use changes on carbon and nutrient cycles, we are developing a reactive transport model that couples hydrologic and biogeochemical processes to microbial functional distributions inferred from site-specific 'omic' data. The objective of the modeling approach is to simulate changes in carbon and nutrient fluxes and aquifer biogeochemistry over longer time periods due to changes in climate and/or land use, while also considering shorter time periods in which water table fluctuations and temperature variations are important.

A 2-D reactive transport model has been developed for the unsaturated-saturated zone of the Rifle site, CO, an alluvial aquifer bordering the Colorado River. Modeling efforts focus on the April through September 2013 time frame that corresponds to the spring snow melt event that lead to an approximately 1 meter rise in the water table followed by a gradual lowering over 3 months. Temperature variations of as much as 10°C are observed at shallow depths (< 1m), while at least some temperature variation (1ºC) occurs as deep as about 7m. A field survey of the microbial populations indicates the presence and activity of chemo(litho)autotrophic bacteria within the saturated zone of the alluvial aquifer.

Model simulations are used to quantify the release of carbon dioxide and consumption of oxygen via abiotic pathways and heterotrophic microbial oxidation of reduced species (Fe(II), S(-2)) and minerals (pyrite). Results indicate that the observed oxygen profiles and/or carbon fluxes cannot be matched by considering abiotic reactions alone. The importance of including microbial contributions from chemo(litho)autotrophic processes (e.g., ammonia, sulfur and iron oxidation) is supported by both field observations and model simulations. Important conclusions from the study are to: (1) include microbially-mediated processes and contributions from the unsaturated zone, and (2) account for seasonal temperature changes to accurately represent lateral and vertical delivery of water and nutrients as well as biogeochemical transformations within the Rifle Flood Plain system.

B31B-0020: Genome-to-Watershed Predictive Understanding of Terrestrial Environments

Wednesday, December 17, 2014

08:00 AM - 12:20 PM, *Moscone West, Poster Hall*

Susan S. Hubbard[1], *Deb Agarwal*[1], *Jillian F Banfield*[1,2], *Harry R Beller*[1], *Eoin Brodie*[1], *Phillip Long*[1], *Peter S Nico*[1], *Carl I Steefel*[1], *Tetsu K Tokunaga*[1], *Kenneth Hurst Williams*[1] *and the Sustainable Systems SFA 2.0 Team (http://esd.lbl.gov/research/projects/sssfa2/), (1)Lawrence Berkeley National Laboratory, Berkeley, CA, United States, (2)University of California Berkeley, Berkeley, CA, United States*

Abstract Although terrestrial environments play a critical role in cycling water, greenhouse gasses, and other life-critical elements, the complexity of interactions among component microbes, plants, minerals, migrating fluids and dissolved constituents hinders predictive understanding of system behavior. The 'Sustainable Systems 2.0' project is developing genome-to-watershed scale predictive capabilities to quantify how the microbiome affects biogeochemical watershed functioning, how watershed-scale hydro-biogeochemical processes affect microbial functioning, and how these interactions co-evolve with climate and land-use changes. Development of such predictive capabilities is critical for guiding the optimal management of water resources, contaminant remediation, carbon stabilization, and agricultural sustainability – now and with global change. Initial investigations are focused on floodplains in the Colorado River Basin, and include iterative model development, experiments and observations with an early emphasis on subsurface aspects. Field experiments include local-scale experiments at Rifle CO to quantify spatiotemporal metabolic and geochemical responses to $O_2$and nitrate amendments as well as floodplain-scale monitoring to quantify genomic and biogeochemical response to natural hydrological perturbations. Information obtained from such experiments are represented within GEWaSC, a Genome-Enabled Watershed Simulation Capability, which is being developed to allow mechanistic interrogation of how genomic information stored in a subsurface microbiome affects biogeochemical cycling.
This presentation will describe the genome-to-watershed scale approach as well as early highlights associated with the project. Highlights include: first insights into the diversity of the subsurface microbiome and metabolic roles of organisms involved in subsurface nitrogen, sulfur and hydrogen and carbon cycling; the extreme variability of subsurface DOC and hydrological controls on carbon and nitrogen cycling; geophysical identification of floodplain hotspots that are useful for model parameterization; and GEWaSC demonstration of how incorporation of identified microbial metabolic processes improves prediction of the larger system biogeochemical behavior.

B31B-0021: MODELING MICROBIAL BIOGEOCHEMISTRY FROM TERRESTRIAL TO AQUATIC ECOSYSTEMS USING TRAIT-BASED APPROACHES

Wednesday, December 17, 2014

08:00 AM - 12:20 PM, *Moscone West Poster Hall*

Eric King[1,2], *Sergi Molins*[1], *Ulas Karaoz*[2], *Jeffrey N Johnson*[3], *Nicholas Bouskill*[1], *Laura A Hug*[4], *Brian C Thomas*[4], *Cindy J Castelle*[4], *Harry R Beller*[1], *Jillian F Banfield*[4], *Carl I Steefel*[1] *and Eoin Brodie*[1], *(1)Lawrence Berkeley National Laboratory, Berkeley, CA, United States, (2)Lawrence Berkeley National Lab, Berkeley, CA, United States, (3)Lawrence Berkeley National Lab, Oakland, CA, United States, (4)University of California Berkeley, Berkeley, CA, United States*

Abstract Currently, there is uncertainty in how climate or land-use-induced changes in hydrology and vegetation will affect subsurface carbon flux, the spatial and temporal distribution of flow and transport, biogeochemical cycling, and microbial metabolic activity. Here we focus on the initial development of a Genome-Enabled Watershed Simulation Capability (GEWaSC), which provides a predictive framework for understanding how genomic information stored in a subsurface microbiome affects biogeochemical watershed functioning, how watershed-scale processes affect microbial function, and how these interactions co-evolve. This multiscale framework builds on a hierarchical approach to multiscale modeling, which considers coupling between defined microscale and macroscale components of a system (e.g., a catchment being defined as macroscale and biogeofacies as microscale).

Here, we report our progress in the development of a trait-based modeling approach within a reactive transport framework that simulates coupled guilds of microbes. Guild selection is driven by traits extracted from, and physiological properties inferred from, large-scale assembly of metagenome data. Meta-genomic, -transcriptomic and -proteomic information are also used to complement our existing biogeochemical reaction networks and contributes key reactions where biogeochemical analyses are unequivocal. Our approach models the rate of nutrient uptake and the thermodynamics of coupled electron donors and acceptors for a range of microbial metabolisms including heterotrophs and chemolitho(auto)trophs. Metabolism of exogenous substrates fuels catabolic and anabolic processes, with the proportion of energy used for each based upon dynamic intracellular and environmental conditions. In addition to biomass development, anabolism includes the production of key enzymes, such as nitrogenase for nitrogen fixation or exo-enzymes for the hydrolysis of extracellular polymers. This internal resource partitioning represents a trade-off against biomass formation and results in microbial population emergence across a fitness landscape. We use this model in simulations to explore the controls on community emergence and impact on rates of reactions that contribute to the cycling of carbon across distinct redox zones of an aquifer.

B31B-0022: Estimating groundwater dynamics at a Colorado floodplain site using historical hydrological data and climate information

Wednesday, December 17, 2014

08:00 AM - 12:20 PM, *Moscone West Poster Hall*

***Jinsong Chen**, Lawrence Berkeley National Lab, Berkeley, CA, United States, Susan S. Hubbard, Lawrence Berkeley National Laboratory, Berkeley, CA, United States and Kenneth Hurst Williams, Colorado School of Mines, Golden, CO, United States*

Abstract Developing a predictive understanding of how hydrological variations impact biogeochemical cycles in terrestrial environments is challenging due to the wide range of processes occurring across vast spatiotemporal scales and due to the uncertainty associated with future climate conditions. In this study, we develop a multi-scale time series model to estimate groundwater dynamics at a floodplain site using historical hydrological data and climate information. Our study is focused at Rifle, CO, where the US DOE Sustainable Systems 2.0 project is developing a genome-to-watershed reactive transport simulation capability and where snowmelt annually delivers a hydrological pulse to the floodplain system that significantly influences the water table and subsurface cycles of carbon and nitrogen. Although long-term predictions of biogeochemical cycling at the site require estimates of hydrological conditions, hydrological data include only a few years of groundwater elevation measurements, with river gage data available from a station located approximately 26 miles upstream.

To project future hydrological conditions at the site, we developed a multi-scale statistical model to combine both datasets. We first analyzed 47 years of hydrological data from the gage station to identify multi-frequency temporal patterns in the river stage and its relationship to climate factors (e.g., precipitation or temperature). We then developed empirical models to downscale the estimated hydrological information to daily discharge and subsequently transform them to groundwater dynamics at the downstream floodplain site. Our model provides a probabilistic estimation that is conditioned to the multi-scale hydrological and climate information. With the developed approach, we retrospectively estimate groundwater dynamics at the site for the past five decades as well as the associated uncertainty. Based on Colorado River Basin climate projections, we also predict mean and extreme hydrological conditions at the floodplain site over the next five decades. The projections are being used as input to watershed reactive transport models to predict how hydrological perturbations influence biogeochemical cycles from the genome through watershed scales.

B33B-0163: Novel Approaches for Delineating and Studying "Hotspots" and "Hot Moments" in Fluvial Environments

Wednesday, December 17, 2014

01:40 PM - 06:00 PM, *Moscone West Poster Hall*

Kenneth Hurst Williams[1], *Matthias Bücker*[2], *Adrián Flores Orozco*[2], *Chad Hobson*[1] *and Mark Robbins*[1], *(1)Lawrence Berkeley National Laboratory, Berkeley, CA, United States, (2)Vienna University of Technology, Department of Geophysics, Vienna, Austria*

Abstract Experiments at the Department of Energy's Rifle, CO (USA) field site have long focused on stimulated biogeochemical pathways arising from organic carbon injection. While reductive pathways and their relation to uranium immobilization have been a focus since 2002, ongoing studies are exploring oxidative pathways and their role in mediating fluxes of C, N, S, and aqueous metals. Insights gained from 'stimulation' experiments are providing insight into analogous natural biogeochemical pathways that mediate elemental cycling in the absence of exogenous carbon. Such reactions are instead mediated by endogenous pools of natural organic matter (NOM) deposited during aggradation of aquifer sediments associated with fluvial processes within the Colorado River floodplain. Discrete lenses of fine-grained, organic-rich sediments enriched in reduced species, such as Fe(II) and iron sulfides have been identified along the active margin of the floodplain. Referred to as "naturally reduced zones" (NRZs), these localities constitute a distinct facies type within an otherwise gravel-dominated, largely NOM-deficient matrix. NRZs represent 'hotspots' of seasonally intense C, N, S, and U cycling during excursions in groundwater elevation. Air bubble imbibition within the capillary fringe is inferred to contribute to seasonally oxic groundwater, with its puntuated, 'hot moment' like impact on redox-mediated reactions exhibiting close correspondence to those induced through the intentional introduction of oxidants. Reactions induce sharp gradients in nitrate and sulfate resulting from elevated rates of nitrification and oxidation of reduced sulfur as dissolved oxygen becomes non-limiting. Given their outsized role in constraining the location and timing of critcal element cycling pathways, delineating the distribution of NRZs across scales of relevance to natural field systems is of great importance. Novel mapping approaches borrowed from the field of exploration geophysics provide one means for identifying such 'hotspots' across a variety of environments where their formation is favored. Drilling activities and deployment of monitoring approaches to study cycling pathways of interest and as a function of hydrologic perturbation may then be performed in a targeted and scientificlally-informed manner.

B33B-0164: Subsurface Carbon Cycling Below the Root Zone

Wednesday, December 17, 2014

01:40 PM - 06:00 PM, *Moscone West, Poster Hall*

Jiamin Wan[1], *Wenming Dong*[1], *Yongman Kim*[2], *Tetsu K Tokunaga*[3], *Markus Bill*[4], *Mark E Conrad*[4], *Kenneth Hurst Williams*[4], *Philip E Long*[5] *and Susan S. Hubbard*[4], *(1)Lawrence Berkeley National Laboratory, Earth Science Divission, Berkeley, CA, United States, (2)Lawrence Berkeley National Lab, Earth Science Division, Berkeley, CA, United States, (3)Lawrence Berkely Natl Lab, Berkeley, CA, United States, (4)Lawrence Berkeley National Laboratory, Berkeley, CA, United States, (5)Lawrence Berkeley National Lab, Chelan, WA, United States*

Abstract Carbon in the subsurface below the root zone is an important yet poorly understood link in the terrestrial C cycle, interfacing between overlying soil and downstream aquatic systems. Thus, the nature and behavior of C in the vadose zone and groundwater, particularly the dynamics of mobile dissolved and suspended aqueous species, need to be understood for predicting C cycling and responses to climate change. This study is designed to understand the C balance (influxes, effluxes, and sequestration) and mechanisms controlling subsurface organic and inorganic C transport and transformation. Our initial investigations are being conducted at the Rifle Site floodplain along the Colorado River, in Colorado (USA). Within this floodplain, sediment samples were collected and sampling/monitoring instruments were installed down to 7 m depth at three sites. Pore water and gas samplers at 0.5 m depth intervals within the ~3.5 m deep vadose zone, and multilevel aquifer samplers have yielded depth- and time-resolved profiles of dissolved and suspended organic and inorganic C, and CO_2 for over 1.5 years. Analyses conducted to determine seasonally and vertically resolved geochemical profiles show that dissolved organic matter (DOM) characteristics vary among three distinct hydrobiogeochemical zones; the vadose zone, capillary fringe, and saturated zone. The concentrations of dissolved organic matter (DOM) are many times higher in the vadose zone and the capillary fringe than in groundwater, and vary seasonally. The DOM speciation, aqueous geochemistry, solid phase analyses, and $d^{13}C$ isotope data show the importance of both biotic and abiotic C transformations during transport through the vertical gradients of moisture and temperature. In addition to DOM, suspended organic C and bacteria have been collected from samplers within the capillary fringe. Based on the field-based findings, long-term laboratory column experiments are being conducted under simulated field moisture, temperature, and geochemical conditions in order to gain more quantitative understanding of the C balance within different hydrobiogeochemical zones.

B33B-0165: Ultraviolet-Visible and Fluorescence Analyses Reveal the Spatial and Seasonal Variability of Dissolved Organic Matter through the Vadose Zone to Groundwater at the Rifle, Colorado River Floodplain Site

Wednesday, December 17, 20140
1:40 PM - 06:00 PM, *Moscone West Poster Hall*

***Wenming Dong**, Jiamin Wan, Tetsu K Tokunaga, Benjamin Gilbert, Yongman Kim and Kenneth Hurst Williams, Lawrence Berkeley National Laboratory, Earth Science Divission, Berkeley, CA, United States*

Abstract Dissolved organic matter (DOM) is a complex and poorly understood mixture of natural organic compounds that play important roles in terrestrial C transport and biogeochemical cycles, and its reactivity makes it sensitive to seasonal variations and longer term climate change. As a component within the LBNL Science Focus Area 2.0, this study is designed to determine the spatial and temporal variability of DOM concentrations and characteristics throughout the vadose zone and groundwater within a semi-arid floodplain at Rifle, Colorado. Three sets of vertically stratified pore water samplers and wells were installed along a groundwater flow transect. These installations allowed acquisition of vertically- and temporally-resolved pore water samples from the vadose zone, capillary fringe, and saturated zone from April 2013 to May 2014. Ultraviolet-visible absorbance (UVA) and fluorescence excitation-emission matrix (EEM) spectroscopy are being applied to trace the changes in DOM characteristics. Initial results indicate that the aromatic C contents (%) of DOM vary with depth and season and exhibit patterns distinct from groundwater. EEM analysis identified fulvic- and humic-like substances as the major fluorescent components of DOM in pore water samples. The concentrations of fulvic- and humic-like matter decreases with depth within the vadose zone, and increases from Spring and Summer to Fall, then decreases in Winter. The trend is consistent with UVA results. Microbial by-product-like components in DOM show higher concentrations in the vadose zone, and decrease from Spring to Winter. Fulvic- and humic-like substances are the only detectable fluorophore components in the groundwater samples. The results from both UVA and EEM suggest that (1) aromatic C or fulvic- and humic-like matter are preferentially adsorbed within shallower sediments during transport; and (2) microbial transformations of DOM composition may occur in the vadose zone, particularly during late Spring and early Summer.

B33B-0166: Using Geochemical Indicators to Distinguish High Biogeochemical Activity in Sediments

Wednesday, December 17, 2014

01:40 PM - 06:00 PM, *Moscone West Poster Hall*

***Amy Marietta Kenwell**, Alexis Navarre-Sitchler, Rodrigo Prugue, John R Spear, Kenneth Hurst Williams and Reed M Maxwell, Colorado School of Mines, Golden, CO, United States*

Abstract A better understanding of how microbial communities interact with their surroundings in physically and chemically heterogeneous subsurface environments will lead to improved quantification of biogeochemical reactions and associated nutrient cycling. This study develops a methodology to predict elevated rates of biogeochemical activity (microbial "hotspots") in subsurface environments by correlating microbial community structure with the spatial distribution of geochemical indicators in subsurface sediments. Statistical hierarchical cluster analyses (HCA) of X-ray fluorescence (XRF), simulated precipitation leachate, bioavailable Fe and Mn, total organic carbon (TOC), microbial community structure, grain size, bulk density and moisture content data were used to identify regions of the subsurface characterized by biogeochemical hotspots and sample characteristics indicative of these hotspots within fluvially-derived aquifer sediments. The methodology has been applied to (a) alluvial materials collected at a former uranium mill site near Rifle, Colorado and (b) relatively undisturbed floodplain deposits (soils and sediments) collected along the East River near Crested Butte, Colorado. At Rifle, 33 sediment samples were taken from 8 sediment cores and at the East River 33 soil/sediment samples were collected across and perpendicular to 3 active meanders. The East River watershed exhibits characteristic fluvial progression and serves as a representative example of many headwater catchments with the upper Colorado River basin. Initial clustering revealed that operationally defined hotspots were characterized by high organic carbon, bioavailable iron and dark colors but not necessarily low hydraulic conductivity. Applying the method to identify hotspots in both contaminated and natural floodplain deposits and their associated alluvial aquifers demonstrates the broad applicability of a geochemical indicator based approach.

B42B-02: Evidence of a dynamic microbial community structure and predation through combined microbiological and stable isotope characterization

Thursday, December 18, 2014

10:50 AM - 11:05 AM, *Moscone West 2005*

Jennifer L Druhan[1], *Markus Bill*[2], *Hsiao Chien Lim*[2], *Cindy Wu*[2], *Mark E Conrad*[3], *Kenneth Hurst Williams*[3], *Donald J DePaolo*[3] *and Eoin Brodie*[3], *(1)Stanford University, Geological and Environmental Sciences, Stanford, CA, United States, (2)Lawrence Berkeley National Lab, Berleley, CA, United States, (3)Lawrence Berkeley National Laboratory, Berkeley, CA, United States*

Abstract The speciation, reactivity and mobility of carbon in the near surface environment is intimately linked to the prevalence, diversity and dynamics of native microbial populations. We utilize this relationship by introducing ^{13}C-labeled acetate to sediments recovered from a shallow aquifer system to track both the cycling of carbon through multiple redox pathways and the associated spatial and temporal evolution of bacterial communities in response to this nutrient source. Results demonstrate a net loss of sediment organic carbon over the course of the amendment experiment. Furthermore, these data demonstrated a source of isotopically labeled inorganic carbon that was not attributable to primary metabolism by acetate-oxidizing microorganisms. Fluid samples analyzed weekly for microbial composition by pyrosequencing of ribosomal RNA genes showed a transient microbial community structure, with distinct occurrences of *Azoarcus*, *Geobacter* and multiple sulfate reducing species over the course of the experiment. In combination with DNA sequencing data, the anomalous carbon cycling process is shown to occur exclusively during the period of predominant *Geobacter*species growth. Pyrosequencing indicated, and targeted cloning and sequencing confirmed the presence of several bacteriovorous protozoa, including species of the *Breviata*, *Planococcus* and *Euplotes* genera. Cloning and qPCR analysis demonstrated that *Euplotes* species were most abundant and displayed a growth trajectory that closely followed that of the *Geobacter* population. These results suggest a previously undocumented secondary turnover of biomass carbon related to protozoan grazing that was not sufficiently prevalent to be observed in bulk concentrations of carbon species in the system, but was clearly identifiable in the partitioning of carbon isotopes. The impact of predator-prey relationships on subsurface microbial community dynamics and therefore the flux of carbon through a system via the microbial biomass pool suggests a diversity of processes that should be considered for inclusion in reactive transport models that aim to predict carbon turnover, nutrient flux, and redox reactions in natural and stimulated subsurface systems.

B42B-05: Beyond The Blueprint: Development Of Genome-Informed Trait-Based Models For Prediction Of Microbial Dynamics And Biogeochemical Rates

Thursday, December 18, 2014

11:35 AM - 11:50 AM, *Moscone West 2005*

Eoin Brodie[1,2], *Eric King*[1], *Sergi Molins*[1], *Ulas Karaoz*[1], *Jeffrey N Johnson*[1], *Nicholas Bouskill*[1], *Laura A Hug*[2], *Brian C Thomas*[2], *Cindy J Castelle*[2], *Harry R Beller*[1], *Jillian F Banfield*[1,2] *and Carl I Steefel*[1], *(1)Lawrence Berkeley National Laboratory, Berkeley, CA, United States, (2)University of California Berkeley, Berkeley, CA, United States*

Abstract In soils and sediments microorganisms perform essential ecosystem services through their roles in regulating the stability of carbon and the flux of nutrients, and the purification of water. But these are complex systems with the physical, chemical and biological components all intimately connected. Components of this complexity are gradually being uncovered and our understanding of the extent of microbial functional diversity in particular has been enhanced greatly with the development of cultivation independent approaches. However we have not moved far beyond a descriptive and correlative use of this powerful resource. As the ability to reconstruct thousands of genomes from microbial populations using metagenomic techniques gains momentum, the challenge will be to develop an understanding of how these metabolic blueprints serve to influence the fitness of organisms within these complex systems and how populations emerge and impact the physical and chemical properties of their environment.

In the presentation we will discuss the development of a trait-based model of microbial activity that simulates coupled guilds of microorganisms that are parameterized including traits extracted from large-scale metagenomic data. Using a reactive transport framework we simulate the thermodynamics of coupled electron donor and acceptor reactions to predict the energy available for respiration, biomass development and exo-enzyme production. Each group within a functional guild is parameterized with a unique combination of traits governing organism fitness under dynamic environmental conditions. This presentation will address our latest developments in the estimation of trait values related to growth rate and the identification and linkage of key fitness traits associated with respiratory and fermentative pathways, macromolecule depolymerization enzymes and nitrogen fixation from metagenomic data. We are testing model sensitivity to initial microbial composition and intra-guild trait variability amongst other parameters and are using this model to explore abiotic controls on community emergence and impact on rates of reactions that contribute to the cycling of carbon across biogeochemical gradients from the soil to the subsurface.

B44B-07: Water and Carbon Fluxes in a Semi-Arid Region Floodplain: Multiple Approaches to Constrain Estimates of Seasonal- and Depth Dependent Fluxes at Rifle, Colorado

Thursday, December 18, 2014

05:30 PM - 05:45 PM, *Moscone West 2004*

Tetsu K Tokunaga[1], *Jiamin Wan*[2], *Wenming Dong*[3], *Yongman Kim*[4], *Kenneth Hurst Williams*[5], *Mark E Conrad*[5], *John Neil Christensen*[5], *Markus Bill*[5], *Boris Faybishenko*[5], *Chad Hobson*[5], *Richard Dayvault*[6], *Philip E Long*[7] *and Susan S. Hubbard*[5], *(1)Lawrence Berkely Natl Lab, Berkeley, CA, United States, (2)Univ of California, Berkeley, CA, United States, (3)Lawrence Berkeley National Lab, Berkeley, CA, United States, (4)Lawrence Berkeley National Lab, Earth Science Division, Berkeley, CA, United States, (5)Lawrence Berkeley National Laboratory, Berkeley, CA, United States, (6)S. M. Stoller, Grand Junction, CO, United States, (7)Lawrence Berkeley National Lab, Chelan, WA, United States*

Abstract The importance of floodplains as links between watersheds and rivers highlights the need to understand water and carbon fluxes within floodplain profiles, from their surface soil, through the vadose zone and underlying groundwater. Here, we present results of field and laboratory measurements conducted to quantify fluxes at a remediated uranium/vanadium mill tailings site on a floodplain at Rifle, Colorado. This semi-arid site has a vegetated, locally derived fill soil that replaced the original milling-contaminated soil to a depth of about 1.5 m. The fill soil overlies about 4.5 m of native sandy and cobbly alluvium containing the shallow aquifer. The aquifer generally drains into the Colorado River and is underlain by low permeability Wasatch Formation shale. Within this system, key issues being investigated include water and carbon fluxes between the vadose zone and aquifer, and CO_2 fluxes through the vadose zone soil out to the atmosphere. Magnitudes of these fluxes are typically low, thus challenging to measure, yet increasingly important to quantify given the expansion of arid and semi-arid regions under changing climate.

The results of field investigations demonstrated that the annual water table rise and fall are driven by snowmelt runoff into the Colorado River in late spring to early summer. Tensiometer data indicate that net recharge from the deeper part of the vadose zone into groundwater occurs later in summer, after water table decline. The effectiveness of summer evapotranspiration in limiting groundwater recharge is reflected in water potentials decreasing to as low as -3 MPa within the upper 1.5 m of the vadose zone. Examination of the historical precipitation record further indicates that net recharge only occurs in years with above-average precipitation during winter and spring. These short intervals of net recharge also facilitate C transport into groundwater because of higher organic C concentrations in the vadose zone. Fluxes of CO_2 measured at the soil surface are consistent with estimates based on season- and temperature-dependent diffusion and respiration within the vadose zone. Thus, fairly predictable seasonal variations in water table elevation, evapotranspiration, and temperature can help constrain estimates of water and carbon fluxes.

H13C-1131: Development of a Sensor for Measuring In Situ Soil Moisture in Continuous Spatial Profile

Monday, December 15, 2014

01:40 PM - 06:00 PM, *Moscone West Poster Hall*

Stephen Farrington[1], *Neal E Van Wyck*[1] *and Kenneth Hurst Williams*[2], *(1)Transcend Engineering, Bethel, VT, United States, (2)Lawrence Berkeley National Laboratory, Berkeley, CA, United States*

Abstract Land-atmosphere interactions are important sources of seasonal climate predictability and soil moisture is a key parameter that influences land-atmosphere interactions in the climate system. Models of land-atmosphere interaction require reliable input of near surface soil moisture conditions to make accurate predictions, yet a widespread deficit persist in monitoring capability with respect to the near surface soil moisture reservoir on land.

A novel sensor technology based on Time Domain Reflectometry as been demonstrated that has the potential to help advance understanding of land-atmosphere interactions by its ability to acquire continuous profiles of spatially heterogeneous near surface soil moisture over distances up to several meters. The Profile Resolving In-situ Soil Moisture Sensor (PRISMS) technology was tested to establish feasibility and performance both in laboratory conditions and in situ at a U.S. Department of Energy Integrated Field Research Challenge Site are presented. Results include comparison to reference methods.

H13H-1210: Predictive assimilation framework to support contaminated site understanding and remediation

Monday, December 15, 2014

01:40 PM - 06:00 PM, *Moscone West, Poster Hall*

Roelof J Versteeg[1], *Marco Bianchi*[1,2] *and Susan S. Hubbard*[2], *(1)Subsurface Insights, Hanover, NH, United States, (2)Lawrence Berkeley National Laboratory, Berkeley, CA, United States*

Abstract Subsurface system behavior at contaminated sites is driven and controlled by the interplay of physical, chemical, and biological processes occurring at multiple temporal and spatial scales. Effective remediation and monitoring planning requires an understanding of this complexity that is current, predictive (with some level of confidence) and actionable. We present and demonstrate a predictive assimilation framework (PAF). This framework automatically ingests, quality controls and stores near real-time environmental data and processes these data using different inversion and modeling codes to provide information on the current state and evolution of the subsurface system. PAF is implemented as a cloud based software application which has five components: (1) data acquisition, (2) data management, (3) data assimilation and processing, (4) visualization and result deliver and (5) orchestration. Access to and interaction with PAF is done through a standard browser. PAF is designed to be modular so that it can ingest and process different data streams dependent on the site. We will present an implementation of PAF which uses data from a highly instrumented site (the DOE Rifle Subsurface Biogeochemistry Field Observatory in Rifle, Colorado) for which PAF automatically ingests hydrological data and forward models groundwater flow in the saturated zone.

H31H-0720: A High Resolution, Integrated Approach to Modeling Climate Change Impacts to a Mountain Headwaters Catchment using ParFlow

Wednesday, December 17, 2014

08:00 AM - 12:20 PM, *Moscone West Poster Hall*

Christine Elizabeth Pribulick[1], *Reed M Maxwell*[1], *Kenneth Hurst Williams*[2] *and Rosemary W H Carroll*[3], *(1)Colorado School of Mines, Golden, CO, United States, (2)Lawrence Berkeley National Laboratory, Berkeley, CA, United States, (3)Desert Research Institute, Reno, NV, United States*

Abstract Prediction of environmental response to global climate change is paramount for regions that rely upon snowpack for their dominant water supply. Temperature increases are anticipated to be greater at higher elevations perturbing hydrologic systems that provide water to millions of downstream users. In this study, the relationships between large-scale climatic change and the corresponding small-scale hydrologic processes of mountainous terrain are investigated in the East River headwaters catchment near Gothic, CO. This catchment is emblematic of many others within the upper Colorado River Basin and covers an area of 250 square kilometers, has a topographic relief of 1420 meters, an average elevation of 3266 meters and has varying stream characteristics. This site allows for the examination of the varying effect of climate-induced changes on the hydrologic response of three different characteristic components of the catchment: a steep high-energy mountain system, a medium-grade lower-energy system and a low-grade low-energy meandering floodplain. To capture the surface and subsurface heterogeneity of this headwaters system the basin has been modeled at a 10-meter resolution using ParFlow, a parallel, integrated hydrologic model. Driven by meteorological forcing, ParFlow is able to capture land surface processes and represents surface and subsurface interactions through saturated and variably saturated heterogeneous flow. Data from Digital Elevation Models (DEMs), land cover, permeability, geologic and soil maps, and on-site meteorological stations, were prepared, analyzed and input into ParFlow as layers with a grid size comprised of 1403 by 1685 cells to best represent the small-scale, high resolution model domain. Water table depth, soil moisture, soil temperature, snowpack, runoff and local energy budget values provide useful insight into the catchments response to the Intergovernmental Panel on Climate Change (IPCC) temperature projections. In the near term, coupling this watershed model with one describing a diverse suite of subsurface elemental cycling pathways, including carbon and nitrogen, will provide an improved understanding of the response of the subsurface ecosystems to hydrologic transitions induced as a result of global climate change.

H43N-1174: Uranium and Strontium Isotopic Study of the Hydrology of the Alluvial Aquifer at the Rifle Former U Mine Tailings Site, Colorado

Thursday, December 18, 2014

01:40 PM - 06:00 PM, *Moscone West, Poster Hall*

John Neil Christensen[1], *Alyssa E Shiel*[2], *Mark E Conrad*[1], *Kenneth Hurst Williams*[1], *Wenming Dong*[1], *Tetsu K Tokunaga*[1], *Jiamin Wan*[1], *Philip E Long*[1] *and Susan S. Hubbard*[1], *(1)Lawrence Berkeley National Lab, Berkeley, CA, United States, (2)Oregon State University, Geology, Corvallis, OR, United States*

Abstract The Rifle Site consists of a floodplain along the Colorado River that was remediated through the removal of surface material underlying former uranium-vanadium mill tailings. The semi-arid (precip. = ~30 cm/year) catchment for the site has an area of ~1km^2. The Rifle Site provides an excellent field laboratory for the study of the fluxes of water and carbon from the vadose zone to groundwater (LBNL SFA2.0, http://esd.lbl.gov/research/projects/sssfa2/). A network of monitoring wells, particularly a set instrumented in the vadose zone, provide the opportunity to closely sample groundwater and vadose zone porewater both in space and time. In order to better understand the spatial and temporal variation of vadose zone interaction with groundwater within the Rifle floodplain and provide constraints for a Rifle hydrological model, we have analyzed the Sr isotopic compositions, $^{234}U/^{238}U$ activity ratios, and $d^{238}U$ of groundwater, vadose zone porewater (sampled through depth-distributed lysimeters) and surface water including the Colorado River. Significant contrasts in $^{87}Sr/^{86}Sr$ and $^{234}U/^{238}U$ allow the identification of different sources contributing to Rifle groundwater, while $d^{238}U$ provides an additional tracer and insights into redox processes.
Vadose zone porewater is characterized by high $^{87}Sr/^{86}Sr$ and Sr concentrations and falls at one end of a mixing line with Rifle groundwater, while upgradient groundwater with lower $^{87}Sr/^{86}Sr$ and Sr concentrations falls at the other end. A mixing model using vadose zone porewater and upgradient groundwater as endmembers suggests that the contribution of vertical recharge through the floodplain increases to ~20% systematically across the floodplain towards the Colorado River. An exception to this pattern is a well located 150m from the river with recent high U concentrations (>300 ppb) and U and Sr isotopic compositions consistent with a 38% vadose zone contribution. U and Sr isotopes show that an irrigation-return ditch that cuts the site near its eastern edge has significant hydraulic connectivity with the aquifer affecting nearby wells and constraining the boundary conditions for the Rifle hydrologic model. Vadose zone porewater has $d^{235}U$ ranging from 0.03 to 0.6‰ reflecting local smear-zone redox processes or the history of ore sources processed at the Rifle Mill.

H54B-06: Monitoring Soil Hydraulic and Thermal Properties using Coupled Inversion of Time-lapse Temperature and Electrical Resistance Data

Friday, December 19, 2014

05:15 PM - 05:30 PM, *Moscone West 3016*

***Anh Phuong Tran**, Baptiste Dafflon, Susan S. Hubbard, Michael B Kowalsky, Tetsu K Tokunaga, Boris Faybishenko and Phillip Long, Lawrence Berkeley National Laboratory, Berkeley, CA, United States*

Abstract Evaluation of spatiotemporal dynamics of heat transport and water flow in terrestrial environments is essential for understanding hydrological and biogeochemical processes. Electrical resistance tomography has been increasingly well used for monitoring subsurface hydrological processes and estimating soil hydraulic properties through coupled hydrogeophysical inversion. However, electrical resistivity depends on a variety of factors such as temperature, which may limit the accuracy of hydrogeophysical inversion. The main objective of this study is to develop a hydrogeophysical inversion framework to enable the incorporation of nonisothermal processes into the hydrogeophysical inversion procedure, and use of this procedure to investigate the effect of hydrological controls on biogeochemical cycles in terrestrial environments.
We developed the coupled hydro-thermal-geophysical inversion approach, using the iTOUGH2 framework. In this framework, the heat transport and water flow are simultaneously modeled with TOUGH2 code, which effectively accounts for the multiphase, multi-component and nonisothermal flow in porous media. A flexible approach is used to incorporate petrophysical relationships and uncertainty to link soil moisture and temperature with the electrical resistivity. The developed approach was applied to both synthetic and field case studies. At the DOE subsurface biogeochemistry field site located near Rifle CO, seasonal snowmelt delivers a hydrological pulse to the system, which in turn influences the cycles of nitrogen, carbon and other critical elements. Using the new approach, we carried out numerical inversion of electrical resistance data collected along a 100 m transect at the Rifle site, and compared the results with field investigations of the soil, vadose zone, including the capillary fringe, and groundwater, as well as temperature and tensiometer measurements. Preliminary results show the importance of accounting for nonisothermal conditions to reliably interpret electrical resistance measurements and to determine hydraulic and thermal properties that influence biogeochemical cycles.