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Subsurface Biogeochemical Research

University Awards

Poster #21-9

From universal scaling for flow resistance in vegetated channels to predicting algal bloom and the evolution of benthic algae in riverine systems at the reach scale

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BER Program: SBR

Project: University Award

The impact of submerged vegetation on nutrients and contaminants distribution in rivers and streams has been generally overlooked in recent multiscale modeling efforts. Yet, submerged aquatic vegetation (SAV), that consists of rooted macrophytes and attached algae, acts as the regulatory layer between many hydrological and ecological functions. SAV plays a pivotal role in fluvial systems by (1) mediating and regulating the transport between surface waters and the hyporheic zone and (2) promoting biodiversity through the creation of spatial heterogeneity in the flow field. One common challenge in modeling flow and transport in vegetated rivers and streams is the lack of predictive models linking vegetation type and morphology with effective transport properties of the vegetative layer itself and its dynamic linkages to its surroundings (i.e. groundwater and surface waters). Furthermore, the impact of environmental conditions such as water temperature, nutrient availability, light, local hydrodynamics and near-bed fluxes on SAV biomass dynamics (e.g., growth, uptake and removal) has been hard to disentangle. While the availability of LiDAR and unmanned aerial vehicle (UAV) data has opened new opportunities to spatially characterize vegetated environments over large scales, it also has demonstrated the startling limitations of existing models in establishing a mechanistic connection between vegetation morphology, its function and coupled response to variable river and environmental inputs. Here we use a combination of analytical and numerical methods to understand the impact of morphologically complex canopies on friction factor and the dynamic coupling between momentum, mass and SAV biomass evolution in the Khors river bent in Montana. First, we discover a universal scaling law that relates friction factor with canopy permeability and a rescaled bulk Reynolds number; this provides a valuable tool to assess habitats sustainability associated with hydro-dynamical conditions [1]. Second, we develop a 3D code, CladoFOAM, in the OpenFOAM framework, to model Cladophora biomass distribution at the 1.5 km long Khors bent of the Clark Fork river in Montana, where extensive measurements of spatiotemporal evolution of Cladophora coverage at the reach scale, as well as seasonal variations of river discharge, nitrogen input, river temperature, light penetration, and daily/nightly variations of respiration rates, are available. The code, which solves a system of 18 coupled PDEs and ODEs, is able to accurately model the yearly vegetation coverage evolution at the reach scale [2].

[1] S. Rubol, B. Ling and I. Battiato, "Universal scaling-law for flow resistance over canopies with complex morphology", Scientific Reports, Accepted, (2018).

[2] Ling, B., S. Rubol, I. Battiato, 'Predicting algal bloom: the evolution of benthic algae in riverine systems', In preparation for Submission to PNAS, (2018).

Poster #21-66

Geologic Structure of the East River Watershed, Elk Mountains, Colorado: A Preliminary View from New Airborne Geophysical Survey Data

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Project Website: <https://minerals.usgs.gov/science/metal-transport-characterization-mineralized-mountain-watershed/index.html>

Geologic controls on groundwater flow, particularly in structurally and topographically complex mountainous terrain, can be difficult to quantify without a detailed understanding of the regional subsurface geologic structure. This structure can influence the magnitude of groundwater flow through the mountain block, which in turn impacts groundwater composition and the flux of metals and nutrients to near-surface ecosystems. The East River Watershed in the Elk Mountains of Colorado is a research area for numerous projects within the Watershed Function Scientific Focus Area, a number of which are directly related to shallow groundwater flow or ecosystem processes that may be influenced by deep groundwater fluxes. In support of these efforts and on-going mineral resource studies at the U.S. Geological Survey, a regional scale airborne electromagnetic, magnetic, and radiometric survey was conducted of the greater East River watershed in 2017. These data give a view of the regional geologic structure that is unprecedented in both resolution and spatial coverage. This presentation will show preliminary data highlighting the geologic structure of the upper few hundred meters underlying the greater East River watershed. From universal scaling for flow resistance in vegetated channels to predicting algal bloom and the evolution of benthic algae in riverine systems at the reach scale

The impact of submerged vegetation on nutrients and contaminants distribution in rivers and streams has been generally overlooked in recent multiscale modeling efforts. Yet, submerged aquatic vegetation (SAV), that consists of rooted macrophytes and attached algae, acts as the regulatory layer between many hydrological and ecological functions. SAV plays a pivotal role in fluvial systems by (1) mediating and regulating the transport between surface waters and the hyporheic zone and (2) promoting biodiversity through the creation of spatial heterogeneity in the flow field. One common challenge in modeling flow and transport in vegetated rivers and streams is the lack of predictive models linking vegetation type and morphology with effective transport properties of the vegetative layer itself and its dynamic linkages to its surroundings (i.e. groundwater and surface waters). Furthermore, the impact of environmental conditions such as water temperature, nutrient availability, light, local hydrodynamics and near-bed fluxes on SAV biomass dynamics (e.g., growth, uptake and removal) has been hard to disentangle. While the availability of LiDAR and unmanned aerial vehicle (UAV) data has opened new opportunities to spatially characterize vegetated environments over large scales, it also has demonstrated the startling limitations of existing models in establishing a mechanistic connection between vegetation morphology, its function and coupled response to variable river and environmental inputs. Here we use a combination of analytical and numerical methods to understand the impact of morphologically complex canopies on friction factor and the dynamic coupling between momentum, mass and SAV biomass evolution in the Khors river bent in Montana. First, we discover a universal scaling law that relates friction factor with canopy permeability and a rescaled bulk Reynolds number; this provides a valuable tool to assess habitats sustainability associated with hydro-dynamical conditions [1]. Second, we develop a 3D code, CladoFOAM, in the OpenFOAM framework, to model Cladophora biomass distribution at the 1.5 km long Khors bent of the Clark Fork river in Montana, where extensive measurements of spatiotemporal evolution of Cladophora coverage at the reach scale, as well as seasonal

variations of river discharge, nitrogen input, river temperature, light penetration, and daily/nightly variations of respiration rates, are available. The code, which solves a system of 18 coupled PDEs and ODEs, is able to accurately model the yearly vegetation coverage evolution at the reach scale [2].

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Poster #21-62

A Last Line of Defense: Understanding Unique Coupled Abiotic/Biotic Processes at Upwelling Groundwater Interfaces

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The shallow interface sediments that line surface water bodies can host beneficial bacteria that naturally filter contaminants from groundwater as it passes through pores on the way to the surface. When water that is low in dissolved oxygen reaches the oxygenated surface water, metal (typically Fe, Mn) oxides may be precipitated within pores and on grain surfaces. These deposits of metal oxides, which are also observed in abundance within mine-impacted watersheds, act as “contaminant sponges” that sorb toxic compounds. However, dissolved oxygen levels in surface and shallow groundwaters are highly dynamic, and if oxygen with shallow interface sediments is decreased, metal oxides may dissolve and their contaminants released. We have been studying interface sediment-related metal oxides in the laboratory and within mountain watersheds in Colorado to: (1) better understand how dissolved metals, carbon, and contaminants pass from groundwater to surface water, and (2) capitalize on the ability of natural systems to adsorb and sequester contaminants.

In Year 1 of our research at the East River SFA we used fiber-optic distributed temperature sensing (FO-DTS) along with hand-held and Unoccupied Aerial System (UAS)-based thermal infrared surveys to locate focused groundwater discharges to the East River corridor, Oh-Be-Joyful Creek, and Coal Creek; the latter two streams being mine-impacted. We found little evidence of direct groundwater discharge to the river over approximately 4 km of the East River; instead the floodplain seems dominated by lateral exchanges through various meander bends and beaver ponds. A subset of these exchange points showed strong metal oxide deposition. These points were sampled for water chemistry, geophysical properties, and vertical flux rates. In contrast, the smaller mine-impacted streams had numerous direct groundwater discharges to surface water of varied type such as focused fracture flow and diffuse flow through organic-rich sediments.

Geophysical measurements may be sensitive to the metal oxides formed on and within anoxic interface sediments. We have performed extensive laboratory analysis of basic thermal and geophysical materials properties of metal oxide-impacted natural and synthetic (controlled coating) sediments. Our preliminary results indicate that the presence of metal oxides does not reliably induce a magnetic susceptibility response, but does modify the electrical polarization of grain surfaces. Electrical and thermal properties are highly influenced by grain size and sediment type. We plan to utilize this lab-based understanding to refine field geophysical techniques for the efficient spatial mapping of anoxic groundwater discharge zones to streams across the East River SFA.

Poster #21-18

Respiration in Hyporheic Zones: Connecting Mechanics, Microbial Biogeochemistry, and Models

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Rivers are the primary carbon and nutrient conveyors of terrestrial ecosystems. River channels however are not simply inert pipelines. They are hotspots for sink and source reactions with magnitudes just as important as the conveyance. Reduced organic carbon, for example, can be extensively respired by bacteria residing in sediment. Although this respiration process is widely known, it has eluded broad quantification and mechanistic prediction. This incomplete knowledge of the fluxes across the land-water-atmosphere continuum is necessary for calculating terrestrial carbon budgets from plot to ecosystem to global scales.

This investigation seeks to develop plot-scale predictive understanding of carbon respiration in the shallow subsurface of riverbeds, the area referred to as the hyporheic zone. It addresses the overarching question of: “What are the physical and biogeochemical factors controlling hyporheic zone respiration of organic carbon and how are these factors inter-related?” The key factors to be tested are: (1) river hydrodynamics and bed morphology, (2) physical heterogeneity of the sediment hydraulic properties, (3) chemical heterogeneity and bioavailability of particulate organic carbon (POC) within the sediment, (4) riverine dissolved organic carbon (DOC) concentration and its bioavailability, and (5) the microbial community structure. The above factors are being analyzed through advanced computational simulations and laboratory experiments based on field observations from the PNNL SBR-SFA.

The general approach to testing hypotheses to the questions above involves novel flume experiments paired with multiphysics simulations which couple turbulent flow in river channels, hyporheic flow in sediments and reactive transport of carbon and nutrients within both domains. Our team has made a few major steps already and these will be reported in this poster. These include: (1) Flume experiments with detailed flow, chemical, and microbial characterization (2) Fully coupled model (one continuous domain) of turbulent open channel flow and porous media flow with reactive transport developed in OpenFOAM.

Based on (1), we found distinct microbial signatures between oxic and anoxic zones of the hyporheic zone in the sediment. The results also show that the microbial community that grew in the flume is similar to those found in natural aquatic settings. From (2), the novel model is able to replicate flow and transport observations from detailed experiments and from models using more primitive coupling schemes. Our incipient efforts in the past few months have shown the potential for upcoming discoveries regarding how carbon is respired in the hyporheic zones of aquatic sediment.

Poster #21-58

Quantifying Subsurface Biogeochemical Variability in a High Altitude Watershed During Winter Isolation

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Project: University Award

Shallow subsurface microbial and geochemical processes in watersheds are dynamic and responsive to seasonal and long-term environmental change. At high elevation or latitude, such changes may occur during winter months when normal sampling is impossible, impractical, unsafe, or may actually alter the processes being studied. Yet accurate modeling of biogeochemical parameters in the subsurface requires sampling that captures events and persistent cold climate trends. Gaps in current models exist where data have not been collected during extended snow or ice covered periods. Our exploratory study will test the hypothesis that during snow cover in the East River (ER) watershed, episodic excursions of microbial community structure and biogeochemical processes and concentrations will fluctuate from values extrapolated from pre- and post- snow time periods. Elemental and microbial cycles will remain active in the aquifer long after the surface has been covered with snow. Melt events will stimulate biogeochemical processes. Our goal is to demonstrate that data collected through these periods will fill gaps and improve reactive transport models of biogeochemical processes in watersheds. We are coordinating with ongoing studies at the ER site especially those that using reactive transport modeling to frame the biogeochemical processes occurring in the watershed. We describe preliminary work conducted to place the specially designed samplers into the East River and the Shumway well in early November 2017 so that sampling over the winter months can begin.

Poster #21-31

Use of Stable Mercury Isotopes to Assess Mercury and Methylmercury Transformation and Transport Across Critical Interfaces from the Molecular to the Watershed Scale

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Project: University Award

Historical and ongoing releases of mercury (Hg) have resulted in a legacy of Hg contamination in streambed sediment, streambanks, and floodplain soils downstream of the Y-12 National Security Complex (Y12), along the flow path of East Fork Poplar Creek (EFPC) near Oak Ridge, Tennessee. Much of the Hg associated with streambed sediments, streambanks, and floodplain soils resides in relatively insoluble fractions, and has thus been considered to have little impact on dissolved total Hg (THg) concentrations. However, recent studies comparing hydrologic discharge and THg flux from Y12 and Lower EFPC suggest that additional dissolved Hg from the hyporheic pore water or groundwater discharge may variably contribute as much as a third of downstream dissolved Hg loads during baseflow conditions. Thus, one of the overarching goals of this project is to use natural Hg stable isotope signatures, imparted by molecular-scale reactions, to gain a more comprehensive quantitative and mechanistic understanding of the processes that supply dissolved Hg to surface water and drive observations of watershed-scale mercury fluxes. To achieve this goal, we are coupling the Hg isotopic composition of dissolved Hg in stream water and in critical subsurface ecosystem compartments (i.e., hyporheic zone, riparian floodplains, and groundwater) with hydrologic flux measurements in four gauged reaches of EFPC. This will enable us to establish an isotope mass balance that assesses the relative importance of dissolved Hg contributed to the stream across these critical interfaces.

During the first half of this project we have: (1) completed more than a full year of ~ monthly baseflow surface water sampling to characterize the seasonal variability in concentration, flux, and isotopic composition of dissolved Hg in each of four gauged reaches of EFPC; (2) installed infrastructure (semi-permanent piezometers) for sampling hyporheic pore water and secured access to groundwater sampling wells in four reaches of Lower EFPC; (3) collected three seasonal sets of high-volume hyporheic pore water and riparian groundwater samples from these four newly instrumented reaches along the flow path; and (4) developed sequential extraction methods for the isotopic analysis of legacy mercury potentially re-mobilized from streambed sediment. Here, we present: dissolved Hg concentration and Hg isotopic composition of all surface water, hyporheic pore water, and riparian groundwater samples analyzed to date; make mass balance assessments regarding legacy inputs of dissolved Hg to the stream water of EFPC; and provide an assessment of our sequential extraction method for the isotopic analysis of legacy mercury sources.

Poster #21-67

Metabolic Constraints of Organic Matter Mineralization and Metal Cycling During Flood Plain Evolution

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Floodplains are poorly understood and dynamic components of the global carbon cycle that are not well represented in Earth system models. Further, they have a dominant influence on the cycling of important metals, such as uranium, within critical transport conduits between surface waters and groundwater. The physical characteristics of floodplains make the hydrology and associated coupled biology and geochemistry particularly responsive to ongoing and impending changes in climate, river management, and land development.

Important controls on carbon cycling within soils and sediments are imparted by mineral/metal associations and microbial metabolic constraints imposed by the respiratory pathway, both of which further serve to control metal fate and transport. Within floodplain soils and sediments, variations in hydrologic state (water saturation) coupled with structured porous media lead to extensive heterogeneity in redox environments and thus metabolic trajectories controlling organic carbon oxidation.

Using a combination of field-scale measurement with micro-scale laboratory experiments, we find that oxygen diffusion limitations lead to heterogeneous redox profiles, shifting microbial metabolism to less efficient anaerobic SOC oxidation pathways. Across the floodplain transect in the East River watershed we are examining, organic carbon bound to Fe(III) (hydr)oxides constitute the most appreciable C (and N and P) phase, particularly in deeper sediments. Additional laboratory incubations demonstrated that, because organic N and P are preferentially bound to easily reducible Fe(III) (hydr)oxides, these nutrients were mobilized under reducing (water saturated) conditions during flooding. Further, within saturated soils of the floodplain, thermodynamic constraints on microbial metabolism result in preferential utilization of organic carbon compounds. In model soils and sediments, we determined the distribution of operative microbial metabolisms and their cumulative impact on SOM transformations and overall oxidation rates within anaerobic microsites. Metabolic profiling shows anaerobic microsites reduced carbon oxidation rates by an order of magnitude relative to aerobic rates, with Fe reduction contributing more than 75% of the overall metabolism. Dissolved oxygen and nitrate alleviate the metabolic constraint and result in rapid utilization of metabolically protected reduced carbon compounds.

Collectively, our results illustrate the combined, and dynamic, impacts of mineral-associations and metabolic controls on carbon and metal fate. The highly variable hydrology of floodplains leads to concomitant changes in biogeochemical processes within soils that ultimately control organic carbon, nutrients, and metal cycles.

Poster #21-50

On Sub-grid Scale Variations of Transpiration

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Project: University Award

In a climate model in which the land surface is resolved typically at 25 km or more, the focus has been on bulk properties of ecosystem function and structure as they affect the atmosphere. Such a gridbox typically comprises a large number of plant species with various traits, as well as subsurface properties such as porosity and depth to bedrock (DTB). With DOE support, we have developed a stochastic parameterization of hydraulic conductivity that takes into account preferential flow through weathered bedrock (Vrettas and Fung, 2015), and applied the Richards Equation with the new parameterization to investigate the impact of subsurface water storage capacity (especially in the weathered bedrock) and rooting structure on the timing and magnitude of transpiration (Vrettas and Fung, 2017). Here we present an application of the approach to a landscape, using a compilation of DTB at 30 arcsec resolution (Pelletier et al., 2016) and distribution of tree species and associated properties. Rooting depth is calculated using estimates of crown volume of each tree species and climate variables (Schenk and Jackson, 2002); species-specific transpiration dependence on climate is taken from Link et al. (2004). Strategies for upscaling the heterogeneous structure and function to gridbox level will be discussed.

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Poster #21-17

Transport and Transformation of Particulate Organic Matter in Permeable Riverbed Sediments

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Project: University Award

Rivers and other inland water systems are key sites of biogeochemical transformation and storage; they are also distinct ecosystems, geomorphological agents and conduits for material transport across continents to the oceans. Biogeochemical activity in rivers is often conceptualized as occurring predominantly in the water column. However, by far the largest amount of biogeochemical activity takes place within the riverbed, either at or just below the surface. This occurs because the concentration of organic matter (OM) and associated microorganisms is several orders of magnitude higher than the concentration in the water column. Such dynamics have fundamental implications for CO₂ and/or CH₄ production and efflux as well as retention and/or release and transport flux of other nutrients (e.g. N, P) associated with POM decomposition.

Current research efforts are focused on quantifying the short-term (< 0.5 day) accumulation of POM in simulated, permeable riverbed sediment. We have examined the transport and accumulation of fresh algal POM in column reactors packed with Hanford sand and fine-grained silt and clay. Additionally in batch experiments, we have determined that isolated humic acids (HA) can also provide electron donating equivalents to drive dissimilatory iron reduction (DIR), while at the same time serving as electron shuttles that accelerate DIR. Evidence of this phenomenon was provided by the overrepresentation of putative genes coding for enzymes that break down complex lignocellulosic material and (to a lesser extent) aromatic compounds in experiments containing HA. The potential for microorganisms to utilize a small but significant portion of HA is consistent with the emerging view of soil organic carbon as a continuum of variably decomposable organic compounds. The next phase of our research will investigate longer-term (2-4 week) decomposition dynamics of POM in permeable sediments under advective flow.

Poster #21-16

Quantifying Distributed Exchanges of Groundwater with the Columbia River – Preliminary Results

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Streams and rivers receive groundwater from their surrounding contributing watersheds to generally increase channel discharge down the river network. The inflow of groundwater is typically invisible to the naked eye, yet the contribution of groundwater, dissolved solutes, and energy has important biogeochemical and ecological impacts on surface waters. The goal of this project is to determine whether there is a clear relationship between the water management activities within and beyond the river corridor (lands that contribute to rivers; i.e., lateral watershed areas) to the fluxes and locations of groundwater inflows to the river channel. We are developing a new approach to identify the locations of, and estimate the fluxes of contributing groundwater (i.e., groundwater inflow to rivers) along the Columbia River. This new approach relies on detecting water quality anomalies along the river bed – especially dissolved oxygen, temperature, and electrical conductivity – indicating locations of groundwater inflows to the channel. Our data collection platform collects these data and GPS position at high frequency (<1 min). River discharge measurements are made upstream and downstream of these groundwater discharge locations. Combined, these field data would then be used to estimate how much water is entering the river from the ground, based on two mixing models. Repeated throughout the irrigation and non-irrigation seasons, these measurements will be used to determine whether there is a relationship between the locations and/or magnitude of fluxes of groundwater inflow to rivers to irrigation activities in the lateral contributing area to each segment of the river. Here we present our findings from our first field campaign to collect data along a segment of the Columbia River, WA in February 2018.

Poster #21-56

Controls of Hydrological Connectivity on Dissolved Organic Carbon Export in a Seasonally Snow-Covered Watershed

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Biogeochemical reactions at the watershed scale release dissolved organic carbon (DOC), a key solute affecting nutrient cycling and surface water quality. Flushing behaviors have been mostly observed for DOC across different watersheds under diverse conditions. However, underlying mechanisms for such flushing behaviors are poorly understood. Our overall goal is to: 1) develop a watershed-scale hydro-biogeochemical model to enable the simulation of DOC and other microbially-mediated processes; 2) use data-model integration to understand key controls of the DOC behavior at the Coal Creek, which is a seasonally snow-covered watershed (53 km²) located in the west central Colorado.

In this work, a physically-based bio module, bioRT-Flux-PIHM, has been developed on the basis of RT-Flux-PIHM. This new bio module adds a Monod-type subroutine to solve for microbially-mediated processes and thus enables us to simulate DOC and DOC-relevant species (e.g. nutrients, and organic-metal complexes) at the watershed scale. This bio module has been verified against the widely used subsurface reactive transport code CrunchTope on soil carbon and nitrogen processes.

The application of bioRT-FLUX-PIHM in the Coal Creek watershed show that hydrologic connectivity largely determines stream DOC dynamics by shifting the dominant flow pathways and the major DOC sources connected to the stream. Under dry and low connectivity conditions, stream DOC is mainly from groundwater with low DOC concentration; under snow-melting season with high connectivity, stream DOC is predominantly composed of soil water with high DOC concentrations. Responsive SOC reaction rate to hydrologic conditions is a key mechanism to maintain a flushing DOC pattern. Groundwater is an indispensable component to reproduce stream DOC dynamics under baseflow conditions. In summary, stream DOC dynamic is controlled by groundwater influx when the watershed is under low hydrologic connectivity (transport-limited); however, it is largely controlled by soil water reaction when the watershed is under high hydrologic connectivity (supply-limited). These results have important implications for understanding and predicting watershed response to changing hydrological conditions and solute export from land to water.

Poster #21-68

Subsurface Carbon Inventories, Transformations and Fluxes Across Gradients in Elevation and Moisture Within an Alpine Watershed

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The interface extending from the top of the soil layer to the bottom of the water table is characterized by dynamic couplings among vegetation, the movement of water and an array of subsurface biogeochemical processes. This complex interface also contains the largest reservoir of terrestrial carbon (C), one that is highly sensitive to shifts in climate, vegetation, and the resulting hydrologic regimes. Within the LBNL SFA East River, CO watershed study site, we are studying belowground respiration and carbon fluxes and their dependence on (1) the timescales and length scales of moisture variability and (2) molecular-level changes in organic matter compositions due to differing plant inputs and climatic drivers. We are further developing modeling approaches that capture the dynamic response to external forcings (*i.e.*, soil moisture dynamics and plant communities).

We have characterized two microcatchment study sites at different elevations and life zones (2950 and 3500 m; upper montane and upper subalpine, respectively) using depth-resolved soil moisture and temperature sensors, soil gas wells and lysimeters paired with repeat surveys of soil CO₂ fluxes, above ground biomass and belowground soil carbon distributions. Using a combination of Fourier transform infrared spectroscopy (FT-IR) and bulk carbon X-ray absorption spectroscopy (XAS), we find substantial variability in organic carbon functional group abundances between sites at different elevations. Soils at lower elevation are predominantly composed of polysaccharides, while soils at higher elevation have more complex distributions, including substantial portions of carbonyl, phenolic or aromatic carbon. Soil CO₂ respiration rates also show complex seasonal patterns across sites, with the majority of CO₂ production in the shallow (*ca.* <40 cm) soil. Peaks in CO₂ production follow precipitation events, with larger pulses of CO₂ production associated with larger rainfall events. However, the relationship between CO₂ production and soil moisture appears complex and highly variable due to the combined effects of both autotrophic and microbial respiration. Incubation experiments utilizing multiple rewetting events also show a complex dependence on soil moisture. A model framework that captures the transition between active and dormant biomass can explain the incubation experiments and will be examined as a tool for partitioning the net belowground fluxes. Collectively, carbon inputs and speciation and their coupling to soil moisture provide fundamental constraints on subsurface respiration dynamics and their potential response to environmental variability.

Poster #21-47

Towards a Better Understanding of Water Stores and Fluxes: Model Observation Synthesis in a Snowmelt Dominated Research Watershed

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BER Program: SBR

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The hydrology of high-elevation, mountainous regions is poorly represented in Earth Systems Models (ESMs). In addition to regulating downstream water delivery, these ecosystems play an important role in the storage and land-atmosphere exchange of carbon and water. Water balances are sensitive to the amount of water stored in the snowpack (SWE) and the amount of water leaving the system in the form of evapotranspiration—two pieces of the hydrologic cycle that are difficult to observe and model in heterogeneous mountainous regions due to spatially variant weather patterns. In an effort to resolve this hydrologic gap in ESMs, this study seeks to better understand the interactions between groundwater, carbon flux, and the lower atmosphere in these high-altitude environments through integration of field observations and model simulations. We compare model simulations to field observations to elucidate process performance combined with a sensitivity analysis to better understand parameter uncertainty. Observations from a meteorological station in the East River Basin are used to force the integrated hydrologic model, ParFlow-CLM. This met station is co-located with an eddy covariance tower, which, along with snow surveys, is used to better constrain the water, carbon, and energy fluxes in the coupled land-atmosphere model to increase our understanding of high-altitude headwaters systems. Preliminary results suggest the model compares well to the eddy covariance tower and field observations, shown through both correct magnitude and timing of peak SWE along with similar magnitudes and diurnal patterns of heat and water fluxes. Initial sensitivity analysis results show that an increase in temperature leads to a decrease in peak SWE as well as an increase in latent heat revealing a sensitivity of the model to air temperature. Further sensitivity analysis will help us understand uncertainty of snow-related and forcing parameters. Through obtaining more accurate and higher resolution meteorological data and applying it to a coupled hydrologic model, this study can lead to better representation of mountainous environments in all ESMs.

Poster #21-69

Phosphorus Speciation in Atmospherically Deposited Particulate Matter and Potential Impact on Terrestrial Soil Nutrient Cycling and Ecosystem Productivity

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Project: University Award

An accepted paradigm of terrestrial ecosystems in temperate climates is that nitrogen (N) rather than phosphorus (P) is the dominant limiting nutrient to plant growth. Recent studies, however, suggest that the anthropogenic release of large quantities of N-oxides into the atmosphere through fossil fuel combustion has greatly enhanced N inputs to ecosystems, such that the bioavailability of P rather than N may now control terrestrial productivity. To investigate P speciation, sources, seasonal changes, and potential bioavailability of atmospherically deposited P to soil in mountain ecosystems, particulate matter (PM) was collected by passive sampling at high elevation sites in the East River Watershed (CO) study area (in collaboration with the LBNL Watershed Function SFA), and at high and low elevation sites in the Southern Sierra Critical Zone Observatory (SSCZO, CA) during two seasonal periods (Sept.-Oct. 2016 and April-Sept. 2017). Sized-fractionated PM samples were analyzed by bulk and microfocussed XANES at the P K-edge. Aqueous extractions of PM were studied by ³¹P NMR. Analysis of lead isotopes provided information about PM sources. Results from linear combination fits of XANES spectra indicated a mixture of organic and inorganic P species, with organic-P dominating samples from high elevation sites at both CA and CO (~80-95% of total P). Fit results showed that organic P was a mixture of either bulk or adsorbed inositol hexakisphosphate (IHP, also known as phytic acid or phytate), commonly derived from plants, and DNA-P, mostly as an adsorbed species. Results from NMR confirmed the presence of DNA-P in the soluble fraction in addition to monoester-P, pyrophosphate, and inorganic orthophosphate. The lower elevation SSCZO site had a higher fraction of inorganic P (~30-45%), mostly as hydroxyapatite or Ca-associated P. For comparison, soil samples collected at the SSCZO sites had concentrations of total P up to three times lower than PM samples, primarily as inorganic P species (Al-phosphate and clay-associated phosphate). Lead isotope ratios indicated strong seasonal differences in long-range PM input from Asian sources to the CO sites, varying from 0 to almost 60% Asian lead between fall and spring, respectively. These results indicate that organic P dominates in high elevation PM samples, and that seasonally variable long-range transport is an important PM source to mountain ecosystems. Identification of DNA-P in PM samples suggests a more reactive and bioavailable form of P than IHP that has not been previously identified as a significant P component of PM.

Poster #21-37

Characterizing Radionuclide Subsurface Transport from Lab to Field Scales Using Multidimensional, Real-Time Imaging Techniques

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Project: University Award

Project Website: <https://www.clemson.edu/centers-institutes/neesrwm/EPSCoR/>

This abstract provides highlights on real-time imaging studies of radionuclide transport performed as part of a DOE Experimental Program to Stimulate Competitive Research (EPSCoR) Implementation grant in South Carolina. Our approach seeks to characterize the time and length scales over which non-equilibrium states are maintained by rate-limiting (or rate-enhancing) reactions between radionuclides and co-reactants due to interactions between physical mass-transfer processes (i.e., flow, advection, diffusion) and (biogeo)chemical reactions. Multidimensional tools capable of real time monitoring radionuclide mobility were used to monitor lab to field scale experiments.

Highlights from several ongoing experimental and modeling studies will be discussed including:

1. *Development of novel 1D and 3D photon based measurement techniques:* Ex-situ, real-time 1D gamma ray analysis, 3D x-ray CT and, Single Photon Computed Tomography (SPECT) techniques have been used to examine Tc-99m transport through porous media. Data have demonstrated accumulation of Tc within reducing zones of heterogeneous redox environments and a very slow release of Tc into the aqueous phase.
2. *Quantifying flow in porous media using x-ray CT:* Transfer of mass between fast flow in macropores and slow flow in the soil matrix is an important control on the fate and transport of solutes. We show that CT imaging can be used to investigate film flow along macropores, non-uniform imbibition from macropores into soils, and complex filling processes that will ultimately be critical for controlling the movement of radionuclides through the soil as well as the reagents controlling the chemical environment.
3. *Examination of uranyl phosphate dissolution facilitated by biogenic ligands:* The influence of nutrient availability, plant roots and plant root exudates on preferential water flow have been examined using 3D x-ray computed tomography (CT) and 2D light transmission experiments. Results indicate that root exudates influence the wetting of soil surfaces and has a significant impact on preferential water flow. Microfluidics and flow-through batch reactor experiments verified mass transfer limitations of citrate associate with the mineral surface as the primary control of uranyl phosphate dissolution.
4. *Observations of radionuclide transport in field lysimeters:* Field based lysimeter studies of Tc-99 and Np-237 these ions are highly controlled by oxidation of initially Tc(IV) and Np(IV) sources. The rate and extent of source term oxidation was examined through measurements of Np and Tc in the lysimeter effluents during field deployment as well as leaching, batch sorption, x-ray absorption spectroscopy, and

electron microscopy techniques after the lysimeters were retrieved from the field.

This material is based upon work supported by the U.S. Department of Energy Office of Science, Office of Basic Energy Sciences and Office of Biological and Environmental Research under Award Number DE-SC-00012530.

Poster #21-38

Visualizing Macropore Flow Mechanisms using 4D X-ray Computed Tomography

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Project: University Award

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Project Abstract:

Transfer of mass between fast flow in macropores and slow flow in the soil matrix is an important control on the fate and transport of solutes. Time lapse X-ray Computed Tomography (CT) scans provide a non-invasive and non-destructive way to examine fate and transport phenomena in a heterogeneous material in 4D (i.e. transient three-dimensional imaging). Infiltration experiments were performed on a reference column of homogeneous soil and on a soil column with a substantial network of desiccation cracks running the length of the soil. The experiments were conducted by continuously dripping water containing a non-reactive NaI tracer at the top of the dry soil; the initial applied flow rate was 0.12 mL/min, but was increased to 0.33 mL/min after approximately 7 hours. Throughout the experiments the columns were located within a preclinical CT scanner (MILabs, Netherlands) and imaged with high resolution (i.e. 80 micron) at 7 minute intervals to visualize the flow pattern and evaluate mechanisms associated with flow in both the macropore and matrix domains. Quantitative, time-lapse images of water content were obtained from signal intensity changes between the dry and wet CT scans for each column.

The homogeneous column demonstrated an infiltration behavior consistent with standard concepts of unsaturated flow in soils. In contrast, however, complex flow behaviors were observed in the column containing the cracked soil. At low infiltration rates, the flow was dominated by film flow through the macropores (i.e., cracks) with comparatively little imbibition from macropore to matrix. At high infiltration rates, the macropores filled with water and a higher imbibition rate occurred within the soil matrix. A variety of features were also observed that demonstrate complex interactions between the macropores and matrix. For instance, water content increases were observed in the matrix prior to activation of macropore flow, which is consistent with the need to increase local matrix pressures above the threshold air entry pressure of the macropore. Also visible were the formation of flow networks where individual macropores were connected via short flow paths in the matrix. Overall, the results show that the wetting of the soil is a complex process reflecting different contributions from downward infiltration through the matrix and lateral wetting from vertical macropores. These complex filling processes will clearly impact the movement of radionuclides through the soil by advection, but they also have implications for the delivery of reagents that control the chemical environment of the soil, which in turn regulates the mobility of radionuclides.

Poster #21-59

Quantifying Dynamic Water Storage in Weathered Bedrock from the Pore to Landscape Scale

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Project: University Award

Many uplands regions are characterized by shallow soils underlain by weathered and fractured bedrock. The extent to which water is dynamically stored in the weathered bedrock region as “rock moisture” has not been systematically explored, yet its misrepresentation in hydrologic and Earth System models may have significant consequences for predicting transpiration fluxes as well as the chemical composition of groundwater and streamflow. Limited case studies have identified that deeply rooted trees can use water stored in weathered bedrock to subsidize soil moisture, particularly in times of water stress, however, further characterization of the moisture dynamics of the weathered bedrock region are needed to quantify ecosystem sensitivity to environmental change. Here, we seek to develop a predictive, geomorphic framework for quantifying landscape-scale rock moisture storage by directly evaluating differences in weathering profile evolution and dynamic water storage across four sites. Using a combination of near-surface geophysics and drilling, we map the weathered bedrock region and quantify the moisture dynamics within it at three sites associated with the Eel River Critical Zone Observatory, and the East River SFA. In the first six months of the study we have initiated the measurement of catchment-scale erosion rate via cosmogenic radionuclide analysis to evaluate how the pace of landscape evolution impacts weathering profile development. Seismic refraction datasets have now been collected across all four sites and reveal differences in the depth and extent of weathering. To directly quantify dynamic rock moisture storage, we are measuring core-scale petrophysical and hydraulic properties of weathered and unweathered bedrock and conducting successive downhole logging in boreholes, where core and boreholes are available. By the end of 2018, core and borehole logging data will be completed at all four sites. Results of successive logging from two of the sites reveals significant differences in the magnitude and spatial distribution of water storage dynamics that should correspond to the hillslope scale seismic profiles. Additionally, field-scale nuclear magnetic resonance (NMR) logging indicates that dynamic water storage may occur in both the rock matrix and fractures. Laboratory analyses of core samples are underway to further investigate how water storage is distributed at the pore scale. By characterizing the pore- to hillslope-scale distribution of water storage in weathered bedrock at four sites and placing the dynamic storage in the context of landscape and weathering profile evolution, we seek to develop a predictive framework for modeling water storage in weathered bedrock and its impact on the hydrologic cycle.

Poster #21-36

Collaborative Research: Natural Organic Matter and Microbial Matter and Microbial Controls on Mobilization/Immobilization of I and Pu in Soil and Water Affected by Radionuclide Release in USA and Japan

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Project: University Award

In collaboration with Japanese Universities, we carried our research targeting natural organic matter (NOM) compounds and microbial processes that are responsible for speciation and fate of different radionuclides in soils from Japan and the USA. NOM is among the key environmental factors that influences the fate and transport of radionuclides in the environment. While this has been known for decades, there still remains great uncertainty in predicting NOM-radionuclide interactions because of lack of understanding of radionuclide interactions with the specific organic moieties within NOM. Furthermore, radionuclide-NOM studies using modeled organic compounds or elevated radionuclide concentrations provide compromised information related to true environmental conditions. Thus, sensitive techniques are required not only for the detection of radionuclides, and their different species, at ambient and/or far-field concentrations, but also for potential trace organic compounds that are chemically binding these radionuclides. GC-MS, ESI-FTICR-MS and AMS techniques developed in our lab permitted us to define how two radionuclides, iodine (I) and plutonium (Pu), form strong bonds with NOM by entirely different mechanisms: I tends to bind to aromatic functionalities, whereas Pu binds to nitrogen (N)-containing moieties, likely, hydroxamate siderophores.

Microbially mediated chelation and incorporation reactions can control a number of radionuclides, leading to retardation or mobilization, depending on whether the carrier compound is in solution or particle-bound as a function of pH or redox conditions of the ambient environment as well as the molecular weight of the carrier itself (Santschi et al., 2017a,b). In a study with RFETS soils, Pu was found enriched in NOM fractions that contained elevated levels of polycarboxylated aromatic and condensed aromatic formulas. These fractions also contained greater abundance of CHON-type COO formulas, than fractions with lower Pu concentrations. N contents increased with the progression of purification and coincided with the trend of Pu concentration (DiDonato et al., 2017).

Based on humic acid (HA) samples from 10 soils collected from around the world, solid state ¹³C nuclear magnetic resonance (NMR), and C, N, and S elemental analysis, binding of low concentrations of Pu (10⁻¹⁴ M) was correlated to the concentration of carboxylate functionalities and N groups in the particulate and colloidal phases. The much greater tendency of Pu binding to colloidal HAs than to particulate HA has implications on whether NOM acts as a Pu source or sink during natural or man-induced episodic flooding (Lin et al., 2017). In a parallel study, uptake of six particle-reactive and/or redox-sensitive radionuclides (²¹⁰Pb, ²³⁴Th, ⁷Be, ⁵⁹Fe, ²³⁷Np and ²³³Pa) by 14 HA extracts was also investigated revealing the capacity of these HAs to bind strongly to these radionuclides, either in particulate or colloidal state of the HA in a mimicked groundwater slurry (Lin et al., 2018).

While the speciation of radionuclides (e.g., I) can be controlled by abiotic factors such as biogenic Mn oxides at low pH (Grandbois et al., 2018b), biotic factors extracellular enzymes, microbial metabolites and microbial processes that alter the chemistry (e.g. pH, redox conditions) of the immediate environment (Yeager et al., 2017). Grandbois et al. (2018a) showed that the activity of soil enzymes, such as oxidases and peroxidases, and microbial biomass (particularly that of the Acintobacteria) were both strongly correlated with uptake of I at environmentally relevant concentrations in forest soils from different regions and continents.

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Poster #21-32

Methylmercury Uptake and Degradation by Methanotrophs: A Hitherto Unknown, but Potentially Important Environmental Process

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BER Program: SBR

Project: University Award

Project Website: <http://emmb.engin.umich.edu/>

The overall goal of this project is to fully characterize a hitherto unknown mechanism of methylmercury degradation performed by aerobic methanotrophs. Previous work in our laboratories has shown that aerobic methanotrophs, through the production of a novel metal chelator called methanobactin, can bind inorganic mercury (Hg[II]), and by doing so, substantially reduce Hg[II] toxicity. We have also shown that methanobactin can bind a much more toxic form of mercury, the neurotoxin methylmercury (MeHg). Recently, the PIs have found that methanotrophs expressing methanobactin are also able to demethylate significant amounts of MeHg. Unlike the canonical organomercurial lyase in Hg-resistant bacteria, methanotrophs take up and degrade MeHg at environmentally relevant pH and Hg concentrations (i.e., picomolar to nanomolar), suggesting that methanotrophs likely play a critical role in controlling net MeHg production and toxicity *in situ*. However, although methanobactin is necessary for methanotrophic-mediated MeHg degradation, it is not sufficient as purified methanobactin binds, but does not degrade MeHg. That is, methanobactin appears to serve as “delivery” mechanism to enable demethylation of MeHg by an as yet unknown process. Given that methanotrophs are ubiquitous, there exists a critical gap in our understanding of mercury cycling as methanotrophs likely play an important, yet poorly characterized role in controlling MeHg concentrations and by extension, MeHg bioaccumulation. To address this fundamental gap, we will characterize: (1) the products of methanotrophic-mediated MeHg demethylation using ¹³C-labeled MeHg; (2) the mechanism of methanotrophic-mediated MeHg degradation using a suite of selective inhibitors as well as construction of mutants where genes potentially involved in MeHg degradation are knocked out, and (3) the role of methanotrophs in MeHg degradation at the mercury contaminated East Fork Poplar Creek (EFPC) site in Oak Ridge, TN.

Publication:

Semrau JD, DiSpirito AA, Gu W, Yoon S. 2018. Metals and methanotrophy. *Appl Environ Microbiol.* E02289-17. doi:10.1128/AEM.02289-17

Poster #21-55

Mechanistic and Predictive Understanding of Needle Litter Decay in Semi-Arid Mountain Ecosystems Experiencing Unprecedented Vegetation Mortality

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Project: University Award

Montane ecosystems within North America are experiencing a prolonged period of ecological stress resulting from large-scale insect infestation that has affected tens of millions of acres of forest. Repercussions are a concern for the local economy, ecological stability, and biogeochemical processes that can influence water resources, ecosystem function, and human health. The goal of this exploratory project is to isolate relative biogeochemical contributions of needle decay from rhizospheric processes in a perturbed forest ecosystem. To query potential mechanistic drivers, fallen needles under lodgepole and spruce trees from the Rocky Mountains of Colorado were harvested from the forest floor and transported to a montane ecosystem in Crested Butte during the Fall of 2016. The collection enabled a focus on needle chemistry variables of beetle-impacted spruce, non-impacted spruce, and non-impacted lodgepole pine. Defined masses of the needles were deployed in quadruplicate at three distinct elevations to observe the effects of temperature, accelerated snowmelt, and needle chemistry on carbon and nitrogen export into the atmosphere and hydrosphere. Over this past year the needles and underlying soil decay horizons were monitored with a focus on gas flux and soil water chemistry. Initial findings suggest that needle chemistry and seasonality influence gas flux with an observed peak in CO₂ production and CH₄ consumption during high moisture summer events. Gas flux above all three needle types was typically more pronounced than the needle-free controls with lodgepole needle deployments displaying the most significant shift. In contrast, aqueous pore water constituents in proximal soil horizons have shown few shifts based on needle chemistry. However, increased concentrations of DOC, TN, and SUVA were observed after induced snowmelt at 10,400' when contrasted with a proximal natural snowmelt plot. These observations support prior work studying enhanced carbon and nitrogen export into adjacent water bodies after snowmelt. Ongoing work focuses on characterizing the needle composition after decay, microbial ecology shifts associated with variables of elevation and needle chemistry and increased resolution of gaseous and pore water measurements during high moisture summer events. This research has implications for carbon and nutrient export that could aid in the prediction of and preparation for shifts of ecosystem function in montane watersheds with respect to water quality, gaseous export, and forest recovery.

Poster #21-33

***AQUA-MER* Aqueous Speciation Database: A Web Resource for Multi-Scale Modeling of Mercury Biogeochemistry**

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Multi-scale geochemical modeling is important for predicting the fate of metals in terrestrial surface and subsurface systems. Typically, experimentally determined stability constants (i.e., $\log K$) are used to calculate speciation profiles and to predict transport and transformations in the environment. However, modeling mercury (Hg) biogeochemistry suffers from a lack of reliable experimental data. For instance, experimentally measured $\log K$ values for Hg(Cys)₂ vary by 10-20 log units. Furthermore, the $\log K$ value for aqueous HgS was not measured directly but was derived by extrapolating the values for CdS and ZnS. Uncertainty in $\log K$ values propagates nonlinearly through speciation models of aqueous chemical systems. Latin hypercube sampling from a normal distribution of $\log K$ values leads to highly skewed distributions of aqueous Hg-containing species concentrations. Thus, if uncertainty is not considered, speciation model output of concentrations deviate away from the modes of the distributions, or values of the highest probability. Quantum chemical calculations can be used to supplement missing thermodynamic data. We have developed protocols to calculate accurate thermodynamic constants for environmentally relevant molecular species. We have developed an aqueous Hg speciation database, *AQUA-MER*, which collects high-quality experimental data adherent to IUPAC standards, accurate computational data, and provides a web interface to perform multi-scale Hg biogeochemical modeling. Currently, the database includes three modules: experimental $\log K$ data, calculated $\log K$ data, and Hg speciation modeling. The Hg speciation module currently uses PHREEQC to calculate aqueous speciation profiles using thermodynamic constants from experimental data, computational data, or both. Further refinement of the database will provide a one-stop website for multi-scale Hg biogeochemistry studies. Future studies will focus on combining the atomistic models with a macroscopic continuum-scale modeling framework to predict the transport and transformation of Hg in the environment.

Poster #21-65

Preliminary Results of 2017 Drilling, Geophysical Logging, Geologic Mapping, and Geochemical Sampling Activities in Redwell Basin, Elk Mountains, Colorado

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Project: University Award

Project Website: <https://minerals.usgs.gov/science/metal-transport-characterization-mineralized-mountain-watershed/index.html>

A host of drilling, sampling, and geophysical/geological data collection activities were performed during summer 2017 in Redwell Basin, an alpine tributary of the East River in the Elk Mountains, Colorado. Redwell Basin contains bedrock with extensive sulfide mineralization that produces both natural and mining-related acid-rock drainage. The central objective of our project is to characterize and quantify controls on the flux of water and metals in the basin's bedrock groundwater flow system. Surface geophysical surveys were conducted using multiple methods including transient electromagnetic sounding, electrical resistivity tomography, total-field magnetics, and relative gravity. Resulting subsurface information aided in the siting of wells. Drilling activities included drilling a bedrock borehole high in the watershed to a total depth of 81 m with nearly complete core recovery, open-hole packer testing to determine permeability at different depths, and installing a multi-level monitoring well in the hole with four different screen depths. A full suite of borehole geophysical logs were also recorded using standard tools, plus acoustic televiewer, full wave form sonic, and heat-pulse flowmeter. Sixteen shallow piezometers were installed to depths <2 m in both colluvium and bedrock (using a hand-held core drill) in groundwater discharge zones. About 40 water samples were collected from piezometers, adits, springs, and streams, and analyzed for major ion and trace element chemistry and stable isotopes of water. A subset was also analyzed for Sr isotopes and age tracers (tritium, sulfur hexafluoride, and noble gas isotopes). Rock samples were collected from the drill core and submitted for permeability/porosity, petrophysical, petrographic, X-ray diffraction, and other chemical analyses. Finally, geological data collection included outcrop mapping of hydrothermal alteration and brittle structures, as well as comprehensive logging of stratigraphy, structures, and mineralogy in the drill core. Acquisition of analytical results and data interpretation are ongoing, and preliminary results will be presented at the meeting.

Poster #21-57

Snowmelt Dynamics Influence the Distribution of Microbial Communities and Carbon Pools in a Riverbed Ecosystem

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The hydrology of upland catchments in the western US is dominated by seasonal snowmelt that generates peak river discharge in spring and early summer, and low flow conditions for much of the remainder of the year. These snowmelt events are tightly linked to large-scale biogeochemical perturbations within such watersheds. Terrestrial organic carbon and other solutes are exported from hillslopes to the river channel, while increases in river discharge alter patterns of hyporheic mixing and solute processing in the riverbed. To investigate how mixing processes across the hyporheic zone affect carbon and metal processing, both discrete sampling and continuous monitoring efforts have been employed around a characteristic meander on the East River, CO.

Depth resolved temperature probes have been used to infer temporal patterns of flux across the sediment-water riverbed interface. Results have revealed strong river water down welling during periods of snowmelt-linked high discharge that contrast with groundwater up-welling signals during base flow. These hydrologic dynamics exert a strong effect on riverbed pore water geochemistry and microbiology.

While more carbon is exported from the catchment during high flow conditions, the chemistry (and therefore lability) of the DOC pool changes significantly across seasonal time scales. During snowmelt and associated high river discharge, river water carbon chemistry is more homogenous. Due to river water down welling, this signal is distributed into riverbed pore fluids up to 60 cm depth. Contrastingly, under low flow conditions when up-welling groundwater has a greater influence in the riverbed, more diverse and potentially labile carbon compounds are detected in both pore fluids and river water. These mixing patterns also have implications for the riverbed microbiome; under up-welling conditions, microbial communities are more depth stratified, while greater depth-resolved mixing of populations occurs when river water penetrates into the riverbed. These coupled geochemical and microbiological shifts likely affect the rate and extent of carbon and metal processing

These observational data are being complemented by ongoing modeling efforts to understand (1) seasonal transport and degradation of different carbon pools in the hyporheic zone of an upland river, and (2) the influence of spatial patterns in hyporheic mixing on pore water chemistry and microbial communities. The data-enabled models will be used to explore scenarios of carbon processing under a changing climate in mountain watersheds, and better understand how hydrology influences the biogeochemical heterogeneity of streambed environments.

Poster #21-15

Microbial Ammonium Cycling is Critical to Nitrogen Transformations in Columbia River Sediments

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The hyporheic zone plays a major role in carbon and nitrogen fluxes in river systems, yet the microorganisms and their metabolic interactions mediating these processes are largely unknown. To address this knowledge gap, we performed metagenomic and metaproteomic analyses on sediment cores spanning depth and vegetative gradients adjacent to the Columbia River. To date we have reconstructed 20 near-complete genomes from the 6 most abundant and active lineages including members of *Nitrospira* (3 genomes), Thaumarchaeota (6 genomes), Actinobacteria (5 genomes), Aciduliprofundum, as well as novel members within the Deltaproteobacteria, Rokubacteria, and Armatimonadetes (3 genomes). Metabolic predictions from these genomes indicated that ammonium is central metabolite interconnecting nearly all the genomes. For instance, Deltaproteobacteria and Armatimonadetes genomes all encode the capacity to degrade amino acids providing a source of ammonium to system. This metabolite can then be oxidized by Thaumarchaeota to nitrite, which is subsequently oxidized to nitrate by *Nitrospira*, and regenerated to ammonium via dissimilatory nitrate reduction by Actinobacteria. Proteins involved in these predicted activities were detected in the metaproteomic data, confirming that active organic nitrogen fermentation, nitrification, and denitrification co-occur in the subsurface environment. Together our data indicate that nitrogen compounds are transformed by a network of specialists, cycling nitrogen in a modular fashion in the hyporheic zone.

Poster #21-34

Organic Carbon Stability During Fe Redox Reactions: Coupling Geochemistry, Microbiology and Field Monitoring

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In the past two years, we have coupled geochemistry, microbiology and field monitoring to study the stability and reactions of soil organic carbon during the redox reactions of iron (Fe) minerals.

Our geochemical analysis showed that organic carbon associated with pure phase iron (Fe) oxide minerals (hematite, ferrihydrite) and natural Fe oxides in soils was released to the solution phase in conjunction with the reduction of Fe(III). When natural soils were exposed to an anaerobic- aerobic transition, organic carbon respiration was negatively linked to the amount of poorly crystalline Fe-oxide-bound organic carbon, but positively with the crystalline Fe-oxide-bound organic carbon. These results suggest that generation of poorly crystalline Fe oxides during the re-oxidation processes potentially can sequester organic carbon. Other experiments showed that under aerobic conditions, binding with ferrihydrite inhibits the bioavailability of labile substrates such as glucose and formic acid.

We also showed the extracted organic carbon can serve as both electron donor and shuttle for the reduction of hematite and ferrihydrite. In the presence of extracted organic carbon, metagenomes from hematite-reducing cultures had an overrepresentation of genes involved in the degradation of polysaccharides and to a lesser extent aromatic compounds, suggesting complex OC metabolism. Genomic searches for the Porin-Cytochrome Complex resulted in matches to *Ignavibacterium/Melioribacter*, DIRB capable of polymeric OC metabolism. These results indicate that such taxa may have played a role in both Fe reduction and decomposition of complex OC in anoxic soils and sediments. Metagenomes from ferrihydrite-reducing cultures also showed enrichment of genes that may have contributed to the degradation of complex OC (i.e., lignocellulose) into simpler organic compounds that can serve as electron donors for Fe reduction.

For the tundra soil organic carbon dynamic monitoring, in situ observations of CH₄ and CO₂ concentrations were undertaken within and above the soils at the Toolik Field Station over a 2- year period. Field observations showed both net oxidation of CH₄ and production of CO₂ in tundra soils, and suggest that fluxes of both species from the soil are subject to different temperature sensitivities and hysteresis effects upon freezing and thawing. The dynamics of greenhouse gas emissions can potentially be linked to the redox fluctuations.

Collectively our project has provided unique integrative understanding about the biogeochemistry of organic carbon during the redox reactions of Fe.