Cover Page

Genomes to Watersheds Scientific Focus Area

LBNL Genomes to Watersheds SFA
Annual Progress Report

For the period July 1, 2014 – June 30, 2015

GENOMES TO WATERSHED

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FY15 DIGITAL PRODUCTS & UPDATES

SFA Overview video

Metabolic Potential Component Video

Watershed Component Video

Rifle Microbes & Contaminants Video

SFA e-Newsletter

1. OVERVIEW, HIGHIGHTS OF REVIEW PERIOD PROGRESS, and ORGANIZATION

Terrestrial environments are an extremely important component of the Earth system: they yield our water resources, support agriculture and ecosystem diversity, serve as the repository for contaminants, and influence our climate. A prerequisite to effective management of terrestrial environments is the ability to accurately predict the macroscopic behavior of these systems – now and with global change. However, the complexity of the system hinders development of such a predictive understanding due to the multitude of interactions occurring among plants, animals, microorganisms, minerals, migrating fluids, and dissolved constituents within a heterogeneous framework across a wide range of scales. Because below-ground terrestrial processes are perhaps the least understood component of terrestrial systems, processes occurring in this large domain present huge uncertainties in the predictive understanding of biogeochemical cycling and system functions.

Launched in the fall of 2013, the LBNL Genomes to Watersheds Scientific Focus Area 2.0, hereafter called the 'SFA 2.0', is a team-based project that focuses on advancing approaches for quantifying and simulating genome-through-watershed scale interactions that govern biogeochemical cycling in complex terrestrial environments. The SFA 2.0 is an ambitious, modeling-driven enterprise focused on interactions and feedbacks within multi-scale, complex, and biologically-based systems - from the genome to the watershed scales (Figure 1). The project is delineated into three 3-year phases, guided by the following challenges:

Science Question: How will climate induced changes in hydrology and vegetation affect subsurface carbon inputs, flow paths, biogeochemical cycling and metabolic potential; how will these processes evolve over time, and what effect will interactions have on watershed biogeochemical functioning?

Grand Deliverable: Development of a genome-enabled biogeochemical watershed simulation capability (GEWaSC), which provides a predictive framework for understanding how genomic information stored in subsurface microbiome affects biogeochemical watershed functioning; how watershed-scale processes affect microbial functioning, and how these interactions co-evolve.

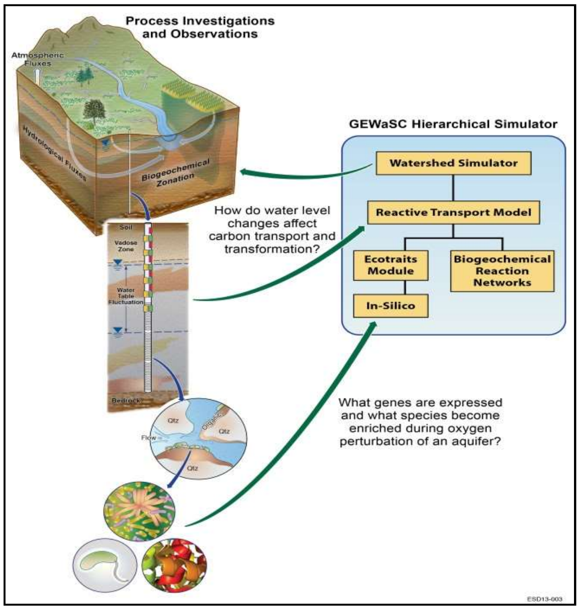


Figure 1. SFA approach to develop a predictive understanding of multi-scale terrestrial environment from the genome to watershed scale.

In addition to our previous research at the Rifle, CO field study site, research during this reporting period has solidified the East River of the Upper Colorado River Basin as a new SFA 2.0 Study Site, which is a mountainous, headwater tributary to the Gunnison and Colorado Rivers (Figure 2). The Colorado is the perhaps the most important Western US River Basin, providing water resources, hydropower, and irrigation for Colorado and many Southwestern states. Many recent studies have documented that the river basin is already being threatened by global change (drought, diminished snowpack, wildfires, and pest outbreaks) that have largely unexplored impacts on the functioning of the river corridor. The Upper Colorado is representative of many mountainous sites worldwide, which globally play an important water resources role (about 60 – 90% of water resources originate from mountains) but which are vulnerable to climate-driven hydrological impacts and associated influence on energy, water, and food for populations far downstream.

The new extension of SFA 2.0 research from the Rifle floodplain to the East River Watershed sites represents a transition across increasing spatial scales, terrestrial environment complexity, and societal

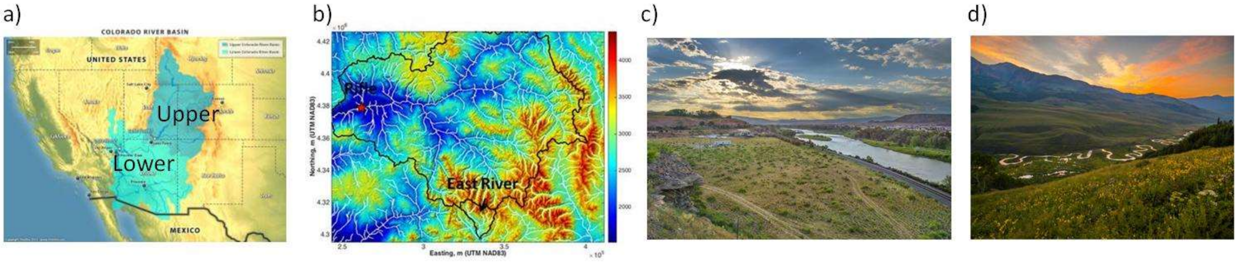


Figure 2. SFA field study site location: a) Colorado River Basin; b) Upper Colorado River Basin, showing locations of Rifle floodplain and East River Watershed focus sites; c) Rifle floodplain; d) East River Watershed

impact of our research. The Rifle floodplain site, which has been extensively characterized and is spatially constrained, has been the focus of early SFA 2.0 research. This site is being predominantly used to meet objectives associated with the first phase of the SFA 2.0 (FY14-FY16), including conducting the first coordinated attempt to gain a predictive understanding of metabolic potential of an entire terrestrial environment, requiring understanding of the genetic, biochemical, and physiological basis of microbial activity in the context of floodplain-wide fluxes and biogeochemical processes, all occurring within a heterogeneous environment. Recent SFA 2.0 research at the Rifle Site (described below) has shown how seasonal snowmelt and perturbation experiments change moisture, oxygen and nitrogen concentrations in the subsurface, which in turn influence carbon transport, biogeochemical transformations, and metabolic potential across the floodplain. The experiments and observations have been used to parameterize and confront the developing GEWaSC capabilities, which have already been successfully demonstrated for predicting metabolic and geochemical in the presence of vertical and lateral heterogeneity across the floodplain site. At the Rifle Site, the SFA 2.0 is now working across bedrock-groundwater-vadose zone-land surface compartments of the floodplain. At the East River Site, we are extending our research to the watershed scale, ad considering bedrock-though-canopy and terrestrial-aquatic coupled hydrological and biogeochemical processes.

The SFA 2.0 is already delivering significant science and technology outcomes. Select examples are mentioned below; these and other advances made during this reporting period are described in Section 2.

- A major scientific discovery during this reporting period is the development and refining of genome reconstruction methods that have now yielded thousands of new genomes at the Rifle Site, identifying major new parts of the tree of life for both Bacteria and Archaea. Notably, these organisms consistently have small genomes and, at least in a subset of cases, small cell size. The research has emphasized the predominance of specific community members under specific field conditions (i.e., chemolithoautrophy during nitrogen and oxygen perturbations) as well as inter-species interactions that mediate biogeochemical cycles. This research has led to several major papers this year, including in Nature and Nature Communications.
- Significant advances have been made in development and testing of modeling frameworks to predict community emergence and its impact on carbon, nutrient, and metal cycling in the subsurface. For example, development of a BioCrunch model included explicit inclusion of ~20 organisms (which were derived and parameterized from literature and metagenomic data) and which catalyzed >30 reactions (such as sulfate reduction and iron oxidation). As an example of the value of including genome-based information in larger-scale models, simulations suggest that neglecting the chemolithoautrotrophic subsurface pathways (which would not have been recognized without metatranscriptomic information) led to an underestimation of dissolved organic carbon exports to the Colorado River by almost 200%, or to a significantly different prediction of carbon cycle dynamics.
- We have documented significant steady-state concentrations of reactive oxygen species (ROS—in this case H_2O_2) along the depth profile of several groundwater wells across the Rifle site. This is a novel observation that is expected to illuminate the importance of ROS in subsurface systems. A kinetic model from related laboratory experiments is being used to interpret these new field results.
- We have found that carbon dissolved in pore waters is only a very small fraction of total soil C inventories. However, high concentrations of dissolved organic carbon (DOC up to 10 mM in some samples), high dissolved inorganic carbon (typically ~ 10 mM), nitrate (several mM in some locations/times), and high salinity are

characteristic of the vadose zone and capillary fringe of the flood plain at Rifle. Soil gas CO_2, O_2 and N_2O concentrations have now been measured for >2 years and exhibit *reproducible* temporal and spatial trends, with the largest fluctuations related to increases in water during peak runoff in the Colorado River stimulating higher levels of sediment microbial activity. Seasonal and depth trends in DOC chemistry are emerging, consistent with progressive *microbial* degradation and sorption of the more aromatic organic carbon fraction.

- We have developed a data-driven approach to combine climate projections with remote stream gauge discharge data to estimate future groundwater dynamics at the Rifle Site. The analysis revealed that the snowmelt-driven water table rise at the Site is expected to occur ~1 month earlier by the end of this Century. As SFA 2.0 Rifle research has already revealed the local importance of the water table rise on nitrogen and carbon cycling, such climate-driven hydrological changes may have important implications for biogeochemical cycles at the Colorado River Basin scale.
- The project has surpassed the 1 millionth data point in the project data management and assimilation archive. Importantly, we are in the process of tightly linking ggKBase with the entire set of Rifle biogeochemistry data which greatly facilitate data mining to reveal heretofore unexplored relationships among genomic and biogeochemical data.

The organizational structure of the SFA facilitates investigations has effectively facilitated progress. The LBNL Genomes to Watersheds SFA 2.0 resides within LBNL's Earth and Environmental Sciences Area and is organized around four process components, GEWaSC, and a Data Management Component (Figure 3). Each component has individual objectives that are being addressed by a team of scientists. The grand SFA challenges are being addressed through participation by all components around common field and laboratory experiments. The SFA team is comprised of ~60 scientists from 6 institutions; a wide range of collaborators complements the SFA expertise and offers significant leveraging (see Section 3). A team retreat was held in October 2014 to continue to share progress and continue to refine the research plan.

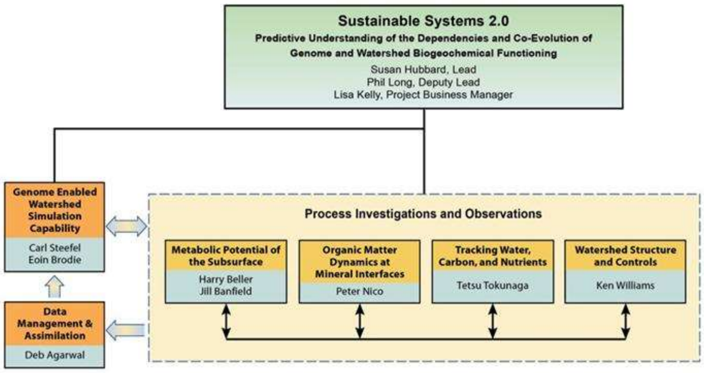


Figure 3. Organizational structure of the SFA 2.0

Excellent research progress of the SFA 2.0 is described in the sections that follow. SFA 2.0 presence is impactful at all major relevant scientific conferences. At the Fall 2014 Meeting of the American Geophysical Union alone, members of the SFA 2.0 gave 25 presentations and were conveners of 5 technical sessions. The SFA has produced 23 publications since the last progress report (See Appendix) and has been involved in multiple outreach activities. The SFA 2.0 has also developed a video library describing the major research components; digital links to these videos are given on the cover page of this report.

2. REPORTING PERIOD RESEARCH PROGRESS

The goals of the SFA are being addressed through advances within and linkage between the six components of the SFA 2.0. Although we report our progress as a function of the components (Sections 2.2- 2.7), much of the progress required linkages and dependencies between the components. To enhance the cross-component coordination, explicit cross-cutting goals and activities were defined to guide FY15 research (Section 2.1). Detailed maps of well locations referred to herein were provided in last year's annual report; an overall view of the floodplain is given in Figure 12.

2.1 Reporting Period Cross-component goals

Cross-component goals are described below and summarized in Table 1. Progress during this reporting period against selected goals is described in subsequent sections as well as in the Appendix. Success for all of the priority required improved accounting of system boundary conditions and their time dependence, especially for fluxes of water and dissolved components, something that has been largely achieved during the reporting period.

Priority Goal 1. Successful demonstration/submission of GEWaSC to simulate Rifle floodplain biogeochemistry through tight metabolic potential linkage.

This goal focuses on inclusion of more realistic carbon reaction network and an ecotrait heterotrophic carbon capability to quantify the role of subsurface microbes in uptake and release of CO_2. At the core of this goal is demonstration of a GEWaSC simulation that directly relies on omics-based data associated with oxygen and nitrogen perturbation experiments.

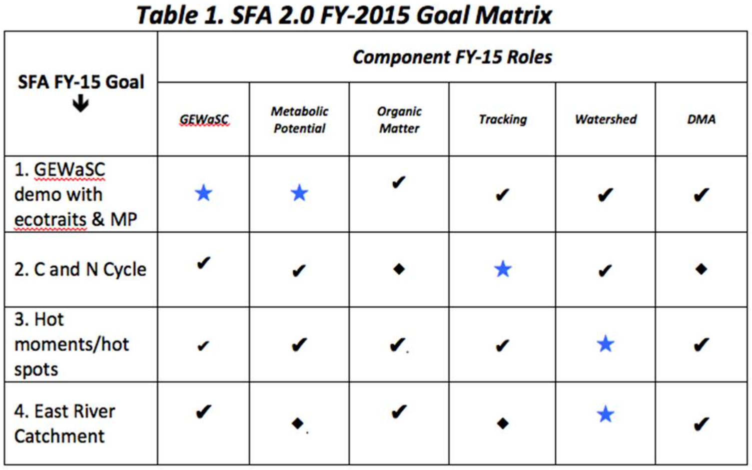


Table 1. SFA 2.0 FY-2015 Goal Matrix

SFA FY-15 Goal ↓	Component FY-15 Roles					
	GEWaSC	Metabolic Potential	Organic Matter	Tracking	Watershed	DMA
1. GEWaSC demo with ecotraits & MP	★	★	✔	✔	✔	✔
2. C and N Cycle	✔	✔	◆	★	✔	◆
3. Hot moments/hot spots	✔	✔	✔	✔	★	✔
4. East River Catchment	✔	◆	✔	◆	★	✔

Table 1: Cross-component goals. Star: components that play a lead role, check: major supporting role; diamond: supporting role

Priority Goal 2. Improved understanding of N and C cycling at Rifle**.** This goal includes consideration of the role of the capillary fringe/saturated zone, and seeks to develop an understanding of the chronically low ammonium concentrations and the transiently high nitrate concentrations observed near a Rifle observation well.

Priority Goal 3. Quantify influence of hot spot/hot moments on Rifle floodplain biogeochemistry.

This goal focuses on quantifying temporal biogeochemical changes associated with observed nitrogen transients following spring snowmelt, and on simulating the influence of (naturally reduced zone) hotspots on floodplain nutrient efflux to river, diversity and the seasonality of microbial community metabolic potential. Importantly, this goal provides an assessment of whether hot moments/hot spots make a difference in the overall biogeochemical cycling (N, C) of the Rifle floodplain.

Priority Goal 4. Initial development of the East River Watershed and associated observations/model

This goal includes preliminary hydro-biogeochemical characterization and development of a flow model that captures transient hydrological events, spatiotemporally resolved geochemical datasets and that will eventually be useful for assessing the ecohydrological implication of a vegetation shift from grass- to shrub-dominated system.

2.2 Genome Enabled Watershed Simulation Capability (GEWaSC)

The GEWaSC component has focused on the development of models at multiple scales and the development of scaling procedures to enable the next generation of nested, multi-scale models. Central to model development has been the ability to: directly connect detailed information on microbial metabolic potential derived from omic studies to biogeochemical reaction networks; condense this information into key microbial features (traits); incorporate this genome-informed trait-based approach into a reactive transport framework; improve the biological pathway complexity of existing reactive transport models; develop an adaptive mesh and model refinement approach for nested mechanistic modeling; integrate reactive transport capabilities into large scale flow and transport models capable of capturing watershed scale heterogeneity.

2.2.1 Linking reconstructed genomes to the reaction network. GEWaSC is critically dependent on new information on the metabolic potential of the Rifle aquifer from vadose zone through the capillary fringe to the saturated zone. Existing reactive transport models are not equipped to take advantage of this new information, so approaches are needed to extract key information and shape its output for use in the next generation of genome-informed reactive transport models. We are building a comprehensive database of curated microbially-mediated reactions relevant to biogeochemical cycling of elements.

The presence of reactions from reconstructed genomes is inferred through a variety of approaches. Reactions are computationally and manually cross-referenced to external resources describing biochemical reactions (KEGG and UniPathway), EC numbers (IntEnz), and protein sequences (UniProtKB). In addition, HMM (InterPro and custom in-house) annotations of the protein sequences indicating the presence of protein domains are being used to directly link reactions to gene predictions.

2.2.2 Trait-based modeling and combined isotopic analysis of nitrogen cycling in the Rifle aquifer.

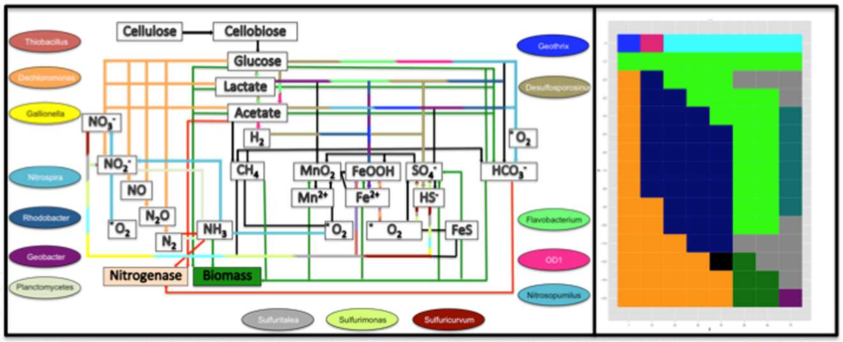
As a next step in the reduction of biological complexity for integration into reactive transport models, we are using a trait-based approach. Many of these traits can be extracted from various 'omic (genomic, transcriptomic, proteomic, metabolomics etc.) information. An initial target of this has been to build upon an existing trait-based N-cycling model to build a more thorough understanding of the nitrogen cycle within the Rifle subsurface. Through on site measurements of nitrate (NO_3), and nitrogen and oxygen isotopes ($\delta^{15}N$- and $\delta^{18}O-NO_3$) and these simple trait-based models, working hypotheses on the important biological pathways for N processing during water table fluctuations are being developed.

Nitrate measurements were taken from pore water extractions through a depth gradient at TT-03 throughout the 2014. As the aquifer transitions from spring to summer the water table rises due to snow melt run-off and NO_3 concentrations decline rapidly indicative of either biological loss or simple dilution. Using measurements of the natural abundance of nitrogen ($\delta^{15}N$- NO_3) and oxygen ($\delta^{18}O-NO_3$) isotopes of NO_3, we distinguished between these two different processes.

In order to determine the potential contribution of heterotrophs and chemolithoautotrophs to nitrogen loss, we have developed a simple trait-based model. This simple model represents the activity of multiple aerobic and anaerobic (denitrifying) heterotrophs, ammonia-oxidizing bacteria and archaea, nitrite-oxiding bacteria and anaerobic ammonia oxidizers (anammox). The model is initialized using O_2 and organic matter (OM) concentrations from the site. Under aerobic conditions, heterotrophic organic matter decomposition results in ammonia release to nitrifiers and nitrate accumulation due to elevated O_2. A rising water table is prescribed through the proportion of water-filled spaces in the sediment, resulting in the rapid consumption of oxygen as consumption exceeds diffusion; shifts in community composition follow with the onset of denitrification. The initial model runs suggest that heterotrophic denitrification is responsible for the bulk of nitrogen loss.

2.2.3 Development of BioCrunch – a genome-informed trait-based model within a reactive transport framework.

Building on these trait-based approaches, we have developed BioCrunch, a genome-informed trait-based model that represents the diversity of microbial functional processes within a reactive transport framework. Microbial dynamics take into account the amount of energy utilized for catabolic/anabolic processes based upon intracellular and environmental conditions with energy dynamically partitioned first into cell maintenance demands and any excess allocated into anabolic reactions. 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. The model therefore explicitly accounts for the growth/death and production and



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enzymatic reaction are shown. Example 2-D simulation results (right) with depth shown on the y-axis and horizontal distance on the x-axis. Because of the complexity of the network and amount of organisms included, colors indicate groups of organisms. For example, green represents cellulose hydrolysis and O_2 dependent S, Fe and NH_3 oxidation along with SO_4^{2-} reduction. Orange depicts SO_4^{2-} reduction and NO_3^- dependent S and Fe oxidation.

degradation of microbes and enzymes as competing sinks for carbon and nitrogen. This internal resource partitioning represents a trade-off against biomass formation and results in microbial population emergence across a fitness landscape. A key feature of BioCrunch stems from its ability to directly incorporate data originating from metagenomics within the metabolic potential component. Genomes derived from metagenomics is used to inform microbial functional process diversity by deriving the organisms and catalyzed reactions utilized in simulations (Fig 4). In addition, metagenomics are used as the basis for parameterizing the large amount of relevant kinetic parameters. For example, genome properties such as codon usage bias can constrain microbial growth rates. To predict community emergence and its impact on carbon, nutrient, and metal cycling, BioCrunch was used to simulate conditions relevant to a non-reducing zone at the Rifle site. ~20 organisms derived and parameterized from literature/ metagenomic data, catalyzing 30+ reactions (e.g. sulfate reduction and iron oxidation) were included. Results showed the pervasiveness of chemolitho-autotrophic processes in the subsurface. For example, *Nitrosopumilus*, an ammonia oxidizer was prevalent in the suboxic region where it was able to utilize its lower affinity for oxygen and corresponding slower growth rates. Nitrate dependent iron and sulfur oxidation was seen throughout the system in accordance with *in situ* metagenomic and transcriptional evidence of *Gallionellaceae* and *Sulfurimonas denitrificans*.

2.2.4 2-D multiphase reactive transport model with improved representation of biogeochemical pathways. As part of the SFA 2.0 modeling efforts, a 2-D reactive transport model was developed to investigate the principal controls on subsurface carbon fluxes in the Rifle floodplain. Previous studies have identified naturally reduced zones (NRZs) in the saturated zone of the Rifle site to be important drivers of biogeochemical fluxes from the dominantly sub-oxic floodplain into the Colorado River. Wavelet analysis of conservative and reactive species at the site suggested that seasonal rise and fall of the Rifle floodplain water table as well as seasonal variation in surface temperatures exert an important control on biogeochemical conditions and reaction rates in the Rifle aquifer.

The vertical 2-D (x-z) model was developed using TOUGHREACT along a transect corresponding to the TT series of wells that includes a NRZ location, and incorporates both the unsaturated and saturated zones. The biogeochemical reaction network includes multiple terminal electron acceptors (TEAs), kinetic and equilibrium mineral precipitation and dissolution, as well as spatially distinct pools of Fe and S minerals and functional microbial populations (Fig. 5). Simulation results were constrained by measurements of water and carbon fluxes along with water table elevation and by isotope and major element chemistry.

Neglecting the chemolithoautrotrophic pathways associated with reduced zones in the simulations resulted in underestimating dissolved organic carbon exports to the river by almost 200%. Simulated groundwater carbon fluxes to the river decreased when averaged over annual water table variations and increased 180% to 3.3 g m^{-2} d^{-1} when averaged over annual temperature fluctuations at the site.

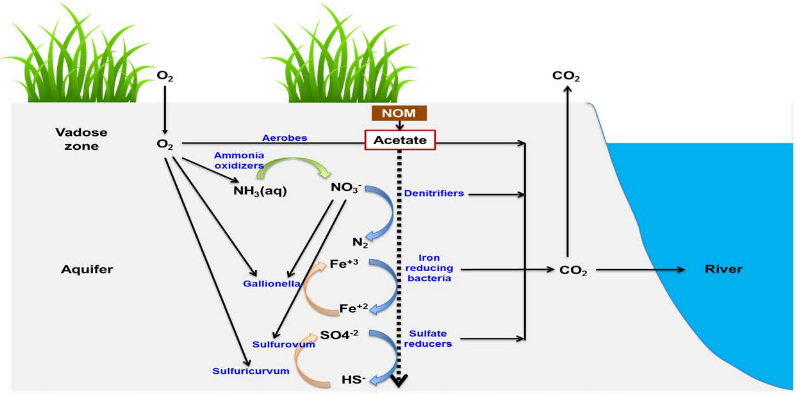


Figure 5. Schematic representation of the biogeochemical reaction network included in model simulations. In this "reduced-order" model, certain microbial species and their functions are explicitly represented in the reaction network (such as Sulfuricurvum as sulfide oxidizer) while the broader diversity of species for other functions (such as sulfate reducers) is modeled by simplified, overall reactions and rates.

2.2.5. 3-D Rifle Flood Plain modeling of carbon and nitrogen fluxes. The goal of the GEWaSC Rifle floodplain modeling is to identify and understand the processes controlling carbon, nitrogen, and oxygen fluxes in the near-surface environment, which includes saturated, unsaturated, and surface zones. The modeling builds on subsurface process and property characterization and reaction networks developed and refined using comprehensive datasets from a series of field studies beginning in 2002. The recent Computational Geosciences article (Yabusaki et al., 2015), "A uranium bioremediation reactive transport benchmark," describes the reaction network and interplay between physical, biological, and geochemical processes in the Rifle aquifer. In addition to the subsurface process characterization, the modeling effort addresses dynamic hydrologic and biogeochemical conditions from the upland watershed and Colorado River and ground surface conditions including precipitation, evapotranspiration, temperature, and relative humidity from the onsite meteorological station.

The Rifle floodplain aquifer is generally anoxic (~0.1 mg/L DO) and nitrate-deficient despite a ~3 m thick overlying vadose zone with near atmospheric levels of gas phase oxygen and high nitrate observations. However, the seasonal rise and fall of the Rifle floodplain water table is associated with an oxygenation event that can last from a few weeks (e.g., June 2013) to a few months (e.g., April-August 2014).

The 3-D floodplain modeling of the 2014 oxygenation event was able to reproduce: the 1) elevated levels of DO in the largely unreactive background biogeofacies,2) maintenance of anoxic conditions and elevated Fe(II) that increases with depth in the NRZ, and 3) leaching of metals from the remnant contaminated vadose zone sediments. Many of the observed behaviors are related to the FeS abundance and depth-dependent distribution. In this case, the background sediments have the lowest FeS abundance and the NRZs have the highest. The essentially complete consumption of elevated DO and production of Fe(II) in the NRZs are consistent with the oxidation of FeS mineral, the abundance of which is higher at depth. The modeling supports a conceptual model of relatively rapid abiotic FeS oxidation during the oxygenation event and slower oxidation (e.g., Fe(II), FeS, ammonium) via chemolithoautotrophy (e.g., Hydrogenophilaceae, Gallionellaceae). The oxidation processes are unsustainable without redox cycling. Modeled anaerobic nitrate (e.g., Gallionellaceae) and sulfate reduction (e.g., Desulfuromonadaceae, Desulfobacteraceae, Desulfobulbaceae) and aerobic respiration (e.g., Comamonadaceae, Rhodocyclaceae) are consistent with the metabolic potential of the metagenome. The heterotrophs responsible for these metabolisms are supported, in part, by labile organic carbon produced by anaerobic fermenters (e.g., Clostridiaceae, OD1-L1). The model also reproduces the observed inhibition of reactions catalyzed by the anaerobes from elevated oxygen.

2.2.6 East River Watershed: Early simulations of coupled hydrological and biogeochemical interactions at the Watershed Scale

The overarching goal of GEWaSC development is to represent heterogeneous hydrological and complex biogeochemical processes in high-resolution, three-dimensional, reactive flow and transport models to predict carbon and nutrient fluxes at the watershed scale. The lower East River system, a high elevation catchment in western Colorado, is rolling-to-mountainous topography with multiple river meanders extending over a distance of 11 km (Fig. 6). Although full build-out of the East River Site will occur during Phase II of the SFA 2.0 project, a hypothesis that we are beginning to test at this site is that the biogeochemical gradients that exist within the hyporheic zone within individual stream meanders significantly impact carbon and nutrient fluxes in the larger East River system, particularly when upscaled over the entire length of the East River Flood Plain.

Figure 6. Aerial view of the Lower East River Catchment, which serves as the initial modeling domain. An up-close view of the stream meanders is given in Figure 2d.

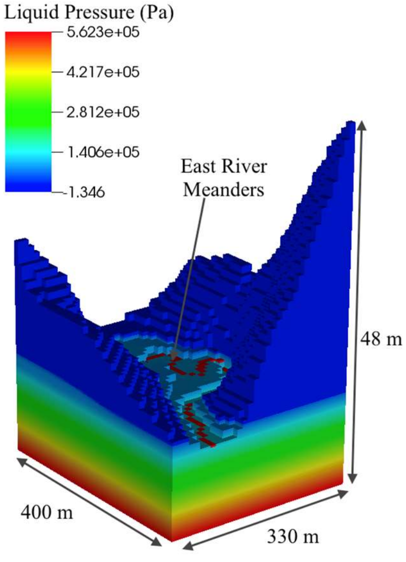


Fig. 7. Model domain showing meandering lower East River and liquid pressure at steady state

To investigate the impact of various processes on the fate and transport of carbon and nutrients in the hyporheic zone over this domain, we developed a complex biogeochemical reaction network and integrated it into the flow and reactive transport code PFLOTRAN (Fig. 7). The biogeochemical reaction network is genome inspired, and it includes multiple carbon and nitrogen species and autotrophic, heterotrophic, and chemolithoautotrophic microbial activity. Also, coupled carbon and nitrogen dynamics are highly uncertain; the prediction of biogeochemical gradients in the hyporheic zone depends on rates of various reactions and extent of hyporheic exchanges resulting from environmental forcing and boundary conditions. Therefore, to predict biogeochemical gradients in the presence of uncertainty, we integrated PFLOTRAN into the iTOUGH, a simulator capable of carrying out inverse modeling and sensitivity analysis. In the lower East River site, results indicate that intra-meander hyporheic zone flow and reaction leads to lateral redox zonation. These redox zones significantly influence the flux of both organic and inorganic carbon into the stream system.

2.2.7 East River Watershed: early projections of hydroecological interactions. The impact of climate-induced changes in vegetation succession on hydrologic processes were investigated in the East River headwaters catchment through development of a 250km^2, 10m resolution watershed transport model using ParFlow. Led by the Watershed Component, 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. The model assessed hydrological changes accompanying worst-case IPCC climate projections and vegetation change scenarios (grassland- to shrub-dominated) as documented through an on-site field study. Changes in available water for evaporation, snow water equivalent (SWE), evapotranspiration (ET) were analyzed along three hillslope transects, with decreases in East River discharge ranging from 16.5-41.3%. The largest decreases were associated with increased ET and snowpack lag, resulting from the shift to a shrub-dominated system combined with increased atmospheric moisture demand and precipitation and melt day transitions under the warming scenario.

2.3 Metabolic Potential

The role of Metabolic Potential is to inform GEWaSC and characterize prevalent metabolic pathways in subsurface microbial communities that mediate carbon and electron flux. During the reporting period, continued excellent progress has been made in genome recovery for and analysis of microorganisms in the aquifer sediment and groundwater, as well as for those that respond to experimental and natural perturbations of the Rifle field site environment (e.g., by addition of oxygen or nitrate).

2.3.1 Metabolic Potential: Summary of recent progress. Subsurface sediments and groundwater are microbially diverse environments that are enriched in organisms some of which are only distantly related to previously encountered bacteria and archaea. In order to access the metabolic potential of the members of these communities we have developed and refined genome reconstruction methods that have now yielded ***thousands of new genomes***. Overall, we estimate that we now have achieved at least reasonably good genomes for almost 30% of the bacteria and archaea that have been detected at the Rifle site. At least a basic metabolic prediction has been accomplished for all of these organisms. Deeper understanding of subsurface microbial communities was gained by conducting perturbation studies that involved addition of naturally occurring electron acceptors (nitrate or dissolved oxygen) and analysis of microbial community gene expression (metatranscriptomics). These studies revealed dominance of chemolithoautrophic activity catalyzed by bacteria that are related to known isolates but that have some unexpected metabolic traits.

We reconstructed and published genome sequences for over 800 bacteria from a large radiation lacking cultivated organisms (average completeness estimated to be 91%). These bacteria are widespread in the Rifle aquifer subsurface, and also in other subsurface environments. Notably, these organisms consistently have small genomes and, at least in a subset of cases, small cell size. Features of these cells include tightly packed spirals inferred to be DNA, few densely packed ribosomes, and a variety of cellular appendages that might enable inter-organism interactions (Luef et al. 2015 Nature Communications).

Many CPR bacterial subgroups have unusual ribosome composition and introns in their single 16S rRNA gene are common. Based on their predicted limited metabolic potential, we infer that these organisms are likely symbionts with ecosystem metabolic impacts associated primarily with fermentation, hydrogen metabolism and in some cases, sulfur metabolism. We designated the large segment of the bacterial domain with which these organisms affiliate as the Candidate Phyla Radiation (CPR; Brown *et al*. Nature, 2015). In addition to genomic sampling the CPR, we reconstructed and partially curated over 2500 genome sequences for other members of the CPR and other bacterial and archaeal lineages (many from the background sediment, O_2 amendment experiment and high and low O_2 groundwater datasets). This genomic dataset is in preparation for publication (Anantharaman *et al*., in prep.) Further, for Archaea specifically, we reconstructed, analyzed and published over 150 genomes, many from a major radiation (referred to as DPANN) from which no isolated organisms have been obtained (Castelle *et al*. Current Biology, 2015). Notably, tens of these genomes are complete (closed, manually curated, no gaps). From the massive genomic dataset we have predicted metabolic capacities and, in some cases, we have integrated the results for specific sample sets or systems to understand which organisms contribute to biogeochemical transformations of interest. An important outcome has been the ability to postulate the metabolic contributions of previously unknown organisms to biogeochemical cycling (Hug *et al*. Environmental Microbiology, 2015).

In general, an intriguing finding of the metabolic analysis is that the novel organisms are responsible for only one or a subset of steps along redox pathways, a result that brings into focus the likely importance of "metabolic handoffs" in the subsurface (Hug *et al*. Environmental Microbiology, 2015). This finding, in combination with the deduction that the CPR and the novel archaea are mostly symbionts, underlines the significance of inter-species interactions and the value of studying microbial communities in their entirety.

Large shifts in community composition occur over space/time/geochemical gradients. We have conducted an analysis of the distribution of a large group of organisms across all available datasets and identified patterns involving similar cohorts that assemble in response to specific geochemical conditions (Hug *et al*. ISME J. 2015). Stimuli (e.g., nitrate amendment, O_2 introduction) led to proliferation of certain microorganisms. In the case of the O_2 injection experiment, environmental change was not readily detectable based on geochemical measurements, but was clearly identifiable by shift in the community structure from consortia dominated by anaerobes to one containing microaerophiles (unpublished).

Genomic reconstructions have been used to understand microbial community responses to environmental perturbations. In the case of the nitrate amendment experiment, proliferation of *Gallionella*-like organisms was noted (discussed below). A reference genome for a closely related strain does not encode nitrate reduction capacity, but this trait is clearly evident in the curated genome from a Rifle groundwater sample and is now emerging as a widespread capacity in these relatively difficult to cultivate bacteria. This example reminds us that phylogeny does not robustly predict physiology, even for closely related organisms. It also reinforces the importance of genome resolution over inference of metabolic capacities from surveys based the 16S rRNA gene. We also showed that ~20% of the bacteria in the Rifle subsurface would likely not be detectable by these surveys due to primer mismatches (Brown *et al*., Nature, 2015).

We conducted a study (in collaboration with the JGI and Illumina) to test the utility of long synthetic reads (previously referred to as Moleculo reads) for metagenomic analysis of complex samples. The approach allowed us to probe the diversity of rare organisms and determine that these were generally similar to organisms detected at higher abundance other samples. The long reads revealed the existence of several highly diverse strain populations that, together, comprised the dominant organism group in the sediments. These organisms were essentially undetectable in short read assemblies. The work was selected for a cover feature of Genome Research (Sharon *et al.* Genome Research, 2015.

In addition to metagenomic analysis, metatrascriptome (community gene expression) analysis was conducted for field-collected samples and provided key insights into the important role of chemolithoautotrophy in mediating the biogeochemical cycling of C, N, S, and Fe in the Rifle subsurface (Jewell *et al.*, in prep.). These field studies were designed to document microbial community response to perturbations caused by amending the aquifer with naturally occurring electron acceptors, namely, nitrate and oxygen. When coupled with metagenomic analysis, metatranscriptome analysis yields extremely valuable information on what metabolic pathways are most active under the tested conditions. Metatranscriptomic analysis revealed pervasive and diverse chemolithoautotrophic bacterial activity in the

Rifle subsurface during the nitrate perturbation. More specifically, chemolithoautotrophic bacteria with very high-ranking genes in sample metatranscriptomes included the following: (1) members of the Fe(II)-oxidizing Gallionellaceae family, (2) anammox bacteria, i.e., planctomycetes capable of anaerobic ammonia oxidation, and (3) strains or close relatives of the S-oxidizing, denitrifying species, *Sulfurimonas denitrificans*. Just these three groups of chemolithoautotrophs accounted for ~80% of the total community gene expression in all post-release samples and ~40% of total gene expression in the pre-release (background) sample. These three groups of chemolithoautotrophs had different temporal patterns of activity throughout the experiment. For example, anammox transcripts maximized in the pre-release sample and Gallionellaceae transcript abundance correlated very strongly with nitrate consumption. There was also clear evidence of different temporal patterns of metabolic activity within the three groups, suggesting that different strains (e.g., two different strains of *Sulfurimonas denitrificans*) occupied somewhat different ecological niches. These data provide key insights into the important role of chemolithoautotrophy in the Rifle subsurface and are being used to inform GEWaSC modeling efforts. Ongoing efforts are being undertaken in the laboratory to isolate a nitrate-reducing *Gallionella* species; the few existing isolates belonging to the Gallionellaceae do not couple Fe(II) oxidation to nitrate reduction, so such an isolate would be a valuable addition to our understanding of iron oxidizers. However, these bacteria are notoriously difficult to cultivate.

Metatranscriptomic analysis is still underway for samples from the dissolved oxygen perturbation, but it is clear that chemolithoautotrophic bacteria were also highly active under those conditions. Relatives of the bacteria that were prevalent and active during the nitrate perturbation were also observed under these conditions. More specifically, in a sample collected 5 to 6 months after the perturbation began, members of the S-oxidizing genus *Sulfuricurvum* and the Fe(II)-oxidizing family Gallionellaceae collectively accounted for more than 50% of community gene expression.

We have been conducting laboratory studies to better understand what natural organic matter fuels heterotrophic microbial communities at Rifle and what genes may be diagnostic of that activity. We have completed the experimental portion of a microcosm study (36 samples) of anaerobic metabolism of organic matter in naturally bioreduced aquifer sediments, involving 5 sampling points for replicated omics (metagenome and metatranscriptome) and biogeochemical measurements (e.g., continuous CO_2 production, H_2, CH_4, acetate, Fe(II), sulfate, NH_4^+, FTIR and other spectroscopic analyses of sediment organic matter). Biogeochemical measurements indicate that the decomposition of native organic matter occurred in different phases, including a pulse of acetogenesis and methanogenesis after 2 weeks of incubation. Metagneomic data have been binned and metatranscriptomic data have been mapped, and analysis is ongoing. This study is a collaboration with the OMD component.

2.3.2 New scientific results or identified gaps that may shift current Metabolic Potential focus.

The diversity, ubiquity and in some samples, high abundance of the CPR bacteria and DPANN archaea raises important questions about their metabolic roles in subsurface microbial communities. Are they pathogens or symbionts? Which organisms are they associated with? Are they specifically associated with specific organisms or generally subsisting on carbon byproducts of other organisms? Are fragments of specific biogeochemical pathways encoded in their genomes significant because they augment pathways of host cells? Are they extracellular partners of bacteria (as was shown for TM7 associated with an actinobacterium by others) or archaea; do they serve, e.g., as phage decoys for their hosts?

Phage genomes obtained in the course of the work to date encode potentially significant genes from the perspective of biogeochemistry (e.g., associated with sulfur cycling) and evolution (e.g., diversity-generating retroelements which, intriguingly, are also common in CPR and DPANN genomes). Phage are also significant from the perspective of cell death and thus carbon turnover. The results motivate new effort to investigate phage-host dynamics; this has been identified as a knowledge gap by the GEWaSC team).

2.4. Organic Matter Dynamics at Mineral Interfaces (OMD)

The OMD component of the SFA is tasked with understanding key mechanisms controlling the chemical form, accessibility, and bioavailability of OM under different geochemical conditions encountered within the Rifle aquifer. In addition to the completed publications listed in the publications section, component team members have three manuscripts currently under review, another four that are in preparation and should be submitted before the end of the fiscal year, and data collected and being analyzed for five more. Recent progress is described below, as a function of key tasks.

2.4.1 Functional group based characterization/classification scheme of OM source types and degradation pathways that can be incorporated into GEWASC.

A NOM extraction scheme was developed using a combination of sequential extraction [water and sodium pyrophosphate (PP) (pH 10)] and purification (dialysis and solid phase extraction (SPE)) in order to isolate different fractions of sediment-associated NOM. Analysis of these different NOM fractions was then carried out by FTIR and ESI-FTICR-MS to allow for comparison of NOM structure and composition both across sites and across fractions for a single location Sediments from the JD well cluster at the Rifle field site from depths ranging between 8.5 to 13 ft bgs, that are located above and below the level of the fluctuating water table were extracted and analyzed. Total extracted OC ranged from 5-17% of the total sediment-bound OC, mostly from the pyrophosphate extraction. SPE recoveries ranged from 21-49% for water extract and 35-47% for PP acid soluble extract. PP acid insoluble >1kD fraction accounted for 33-66% of PP-extracted OC. Only JD-06- 12’ and 13’ samples were visibly reduced. JD-04-8.5’ has similar OC concentrations as JD06-12’, 13’, but 8.5’ is above the seasonally fluctuating water table and is oxidized. Figure 8 shows the FTIR spectra of the different isolated OM fractions from two different sediment depths. C-H peaks are highest in MQ-SPE and lowest in PP acid insoluble >1kD fractions. Principal component analysis performed on the entire set of IR spectra shows separation between different fractions and separation between the two wells. However, the largest differences are noted between fractions rather than between depths.

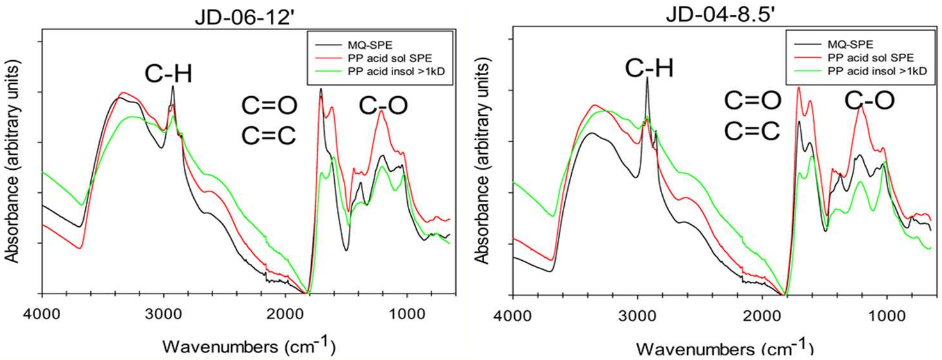


Figure 8: Freeze-dried NOM samples (MQ-SPE, PP acid soluble SPE, PP acid insoluble >1kD) were analyzed by ATR using a diamond crystal and liquid N2-cooled MCT/A detector. Spectra were ATR and baseline-corrected.

More detailed analysis across samples, including peak-fitting of IR spectra and interpretation of FTICR-MS data, is ongoing. Using this combination of analytical techniques we can probe the variation in NOM chemical composition and mineral association across different biogeochemical regimes and assess the potential reactivity of various NOM pools. In combination with targeted field and laboratory experiments, this information can be used to determine key NOM characteristics to consider in modeling the biodegradation, transformation, and flux of carbon under changing conditions.

2.4.2 Quantitative assessment of ROS impact on carbon cycling and shuttling in lab test system with some preliminary field data/test.

Excellent progress has been made on this task this year, with successful efforts in both the laboratory and field. The laboratory work has documented the important catalytic activity of a coupled Fe, ROS cycle to catalytically oxidize ‘lignin-like’ organic functional groups under field pH’s and concentrations. Summary results are presented in Figure 9 showing that 500nmol of Fe can oxidize 10μmol of methoxyhydroquinone, i.e. 20x the amount of Fe, within 2 hrs. These results show that ubiquitous dissolved metals such as Fe play an important role in abiotically transforming organic matter and that reactions with organic matter can maintain steady-state concentrations of Fe(II) in solution in spite of the presence of molecular oxygen. A kinetic model has been built to explain these results, solid line figure Y. This model can now be used to explore the quantitative importance of this process under different geochemical conditions. It can also be incorporated into the larger modeling effort where appropriate.

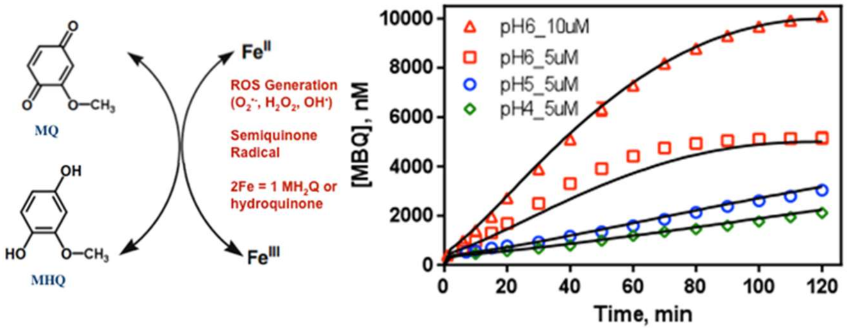
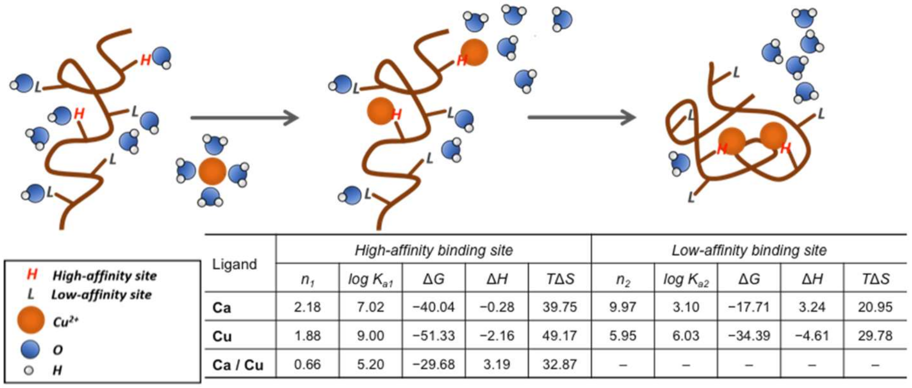


Figure 9. Left: Schematic of Fe catalyzed oxidation of 'lignin-like' methoxy-semiquinone (MHQ) to methoxy-quinone (MQ). Right: Kinetic plots showing that 500 nmol of Fe can catalytically oxidize 10micromol of MBO within two hours.

The fieldwork under this task involved documenting significant steady-state concentrations of H_2O_2 along the depth profile of several groundwater wells across the Rifle site. To the best of our knowledge, this is a completely novel observation and will have a dramatic impact on the understanding of the importance of ROS in subsurface systems. The kinetic model from the laboratory experiments can be used to interpret the field results.

2.4.3 Stability of 'mineral protected' organic matter (OM) under changing spatiotemporal conditions.

A first experimental dataset associated with this topic was generated last year, in which OM from Rifle materials was released into OM-free artificial groundwater. Measurements associated with the simple disequilibrium perturbation demonstrated the strong buffer influence of the mineral phase on OM concentrations in as much as the OM concentration reached a stable concentration within approximately one day and then stayed constant for over >30 days. Although during this time, changes in the OM EEMS spectra were observed, raising questions regarding the nature of chemical changes in OM in spite of the constant concentrations. Progress on this task this year has focused on continued data interpretation of previous experimental results. With the generation of a tentative interpretation of oxidation of lignin-like functional groups accounting for the changes in EEMS signal. The follow up experimental activities for this task this year are scheduled for the last quarter of this fiscal year and are therefore starting up now. They will focus on exploring further perturbations, other than OM free water, on the release of OM from Rifle sediment. In addition, the opportunity has arisen to match these activities with a collaborating field effort to look at OM release as a result of simple chemical disequilibrium conditions in the field.



Ligand	High-affinity binding site					Low-affinity binding site				
	n_1	log K_{a1}	ΔG	ΔH	TΔS	n_2	log K_{a2}	ΔG	ΔH	TΔS
Ca	2.18	7.02	−40.04	−0.28	39.75	9.97	3.10	−17.71	3.24	20.95
Cu	1.88	9.00	−51.33	−2.16	49.17	5.95	6.03	−34.39	−4.61	29.78
Ca / Cu	0.66	5.20	−29.68	3.19	32.87	–	–	–	–	–

Figure 10: Metal binding to standard OM and OM from Rifle is entropy-driven owing to water desolvation and hydrophobic effect and likely impacts organic matter bioavailability by blocking functional groups and driving aggregations.

2.4.4 Correlation between thermodynamics of mineral-om surface sorption and bioavailability.

During this reporting period, research on this task has focused on using isothermal titration calorimetry to quantify the interaction between Ca and Cu with a standard natural organic matter (Suwannee River) and

OM isolated from the Rifle field site. The results show a strong thermodynamic driving force for association of both metals with both organic matters. Somewhat surprisingly, the majority of that driving force is entropic rather than enthalpic. This is likely do to the release of solvated waters and associated ion cloud as a result of close metal binding, see figure 10. Supporting work with AFM has shown strong aggregation of the OM as an impact of complexation by calcium. These results are an important step in building a mechanisms understanding of how and why metal association with organic matter can render otherwise decomposable functional groups stable over long periods of time. Further experiments are now being planned with members of the metabolic potential component to correlate the strength of the interactions, with the degree of aggregation with the decomposability of the OM by rifle microbial consortia. If successful, this work would create a powerful new link between mechanistic chemistry and metabolic activity of subsurface microbial communities.

2.4.5 Continued method development of FT ICRMS, and EEMS. We have continued to work with collaborators at EMSL to develop the use of FT ICR MS for analysis of subsurface OM samples. Preliminary attempts at analysis showed that the standard sample handling and data acquisition approaches were inadequate for OM samples like ours, likely due to high concentrations of complex metal ions associated with the OM. Issues associated with the technique will be explored under the currently pending EMSL proposal mentioned above. Analysis of the MQ-SPE extracts showed similar distributions of functional units with the exception of a greater proportion of sulfur containing groups in the JD-06, 12' sample, likely as a result of being from a more reducing environment within the profile, and emphasizing the importance of S containing organic functional groups under reduced conditions.

2.4.6 New scientific results or identified gaps that may shift current OMD focus. The results from the metal complexation experiments showing the dramatic aggregation impact of complexation of Ca will lead to a new set of experiments with the metabolic potential as described above. In addition, once the field drilling at the East River Site beginnings we will turn greater attention to understanding the sediment associated OM in the context of similarity or difference from that at Rifle. The novel observation of H_2O_2 profiles within Rifle wells will be further explored to quantify the importance of this process on the OM cycling in the subsurface.

2.5 Tracking Water, Carbon and Nutrients

The overall goal of the Tracking Component is to understand subsurface fluxes and transformations of carbon, nutrients, and other components, and how they depend on fluxes of water. Information and understanding gained within Tracking provides input to GEWaSC and other Components, and will help improve predictions on subsurface biogeochemical responses to climate change. Current activities focus on the Rifle Site, where understanding of vadose zone-groundwater interactions is being developed. Recent progress is described below as a function of key tasks.

2.5.1 Rifle field-based insights on water and carbon fluxes. Through partnership with the Watershed Component, hydrobiogeochemical measurements and samples are providing the basis for understanding atmosphere-vadose zone-groundwater interactions. Two new monitoring sites were installed along the existing TT transect in order to better characterize fluxes within the Rifle floodplain. Hydraulic potential profiles are indicative of slow vadose zone recharge in areas closer to the river (TT03 and TT05), and much lower (often zero) recharge through the more upland sites (TT02, TT04, TT01). Soil CO_2 fluxes into the atmosphere are strongly seasonal. Directly measured surface soil CO_2 fluxes are generally consistent with diffusive flux calculations based on vadose zone CO_2 concentration profiles, with the latter indicating important contributions from deeper vadose zone/capillary fringe respiration.

2.5.2 Rifle field pore water and gas sampling and sample analyses. In order to understand the depth and seasonal variations of C, N, and nutrients, the depth-resolved pore water and pore gas samples have been collected every 2-4 weeks through the past year. Although C dissolved in pore waters are only very small fractions of total soil C inventories (Figure 11), high concentrations of dissolved organic carbon

(DOC up to 10 mM in some samples), high dissolved inorganic carbon (typically ~ 10 mM), nitrate (several mM in some locations/times), and high salinity are characteristic of the site vadose zone and capillary fringe. Soil gas CO_2, O_2 and N_2O concentrations have now been measured for >2 years and exhibit reproducible temporal and spatial trends, with the largest fluctuations related to increases in water during peak runoff in the Colorado River stimulating higher levels of soil microbial activity. Seasonal trends in DOC, and depth trends in DOC chemistry are emerging, consistent with progressive microbial degradation and sorption of the more aromatic organic carbon fraction. These data are regularly uploaded onto the SFA database.

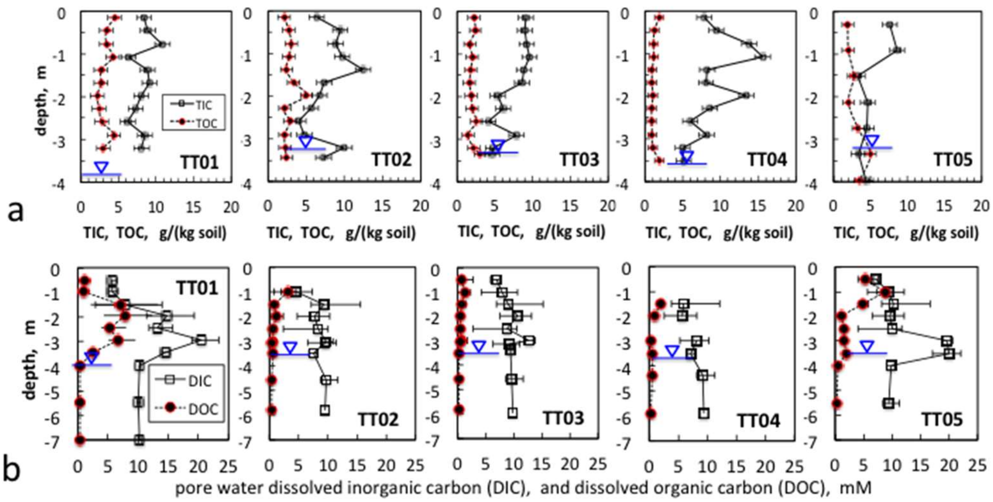


Figure 11. Carbon inventories in profiles along the TT transect. **a.** Total inorganic C and total organic C profiles in sediments. **b.** Pore water conc. of organic and inorganic carbon.

2.5.3 Rifle Strontium isotope signatures. Sr isotopic analyses of Rifle groundwater and vadose samples indicate a contribution of vadose porewater to groundwater of up to 30% (locally in the vicinity of SY08), with an average vadose contribution over the floodplain of ~10%. In this period, independent data analyses (meteorological, salinity) support an average recharge from the vadose zone to the Rifle aquifer of about this magnitude. The Sr isotope model results provide snapshots of the spatial distribution of the magnitude of infiltration across the Floodplain. Comparison of these maps with the Watershed Component's Rifle microtopographic map demonstrates the link between topography and infiltration to groundwater. Locations where the contributions of vadose porewater to groundwater are the greatest generally occur in the lowest part of the site where ponding occurs with greater frequency. Time series of pore water $^{87}Sr/^{86}Sr$ profiles from the TT sites are continuing to be developed to better understand interactions between recharge and seasonal water table fluctuations.

2.5.4 Rifle Uranium isotope signatures. The Spring 2014 water table rise produced a "Hot Moment" at SY02, and coincided with a higher rate of sampling than the previous year. We captured significant excursions in U concentration (peaking at over 700 ppb) and other constituents (Ca, Sr, sulfate, Fe, nitrite/nitrate, etc) accompanied by excursions in $^{87}Sr/^{86}Sr$, ($^{234}U/^{238}U$), and $d^{238}U$ indicating an anthropogenic source of U in the local vadose zone. Our research into the historical record revealed that contamination was left under fill just adjacent to Hwy 6, and that the water table elevation at which the U excursions occurred corresponds to the depth of the contamination. The implication is that the SY02 excursion represents an important U source for plume persistence, perhaps more significant than NRZ's. A similar situation pertains to SY08/TT1 but with an isotopically distinct source of U. These sources provide a semi-natural tracer of groundwater flow across the site, and we continue to monitor downgradient wells for the appearance of these distinct U compositions (as well as capturing this year's excursion in SY02). For the TT wells we have continued to build time series of vadose profiles of $^{234}U/^{238}U$ and now $d^{238}U$ to capture the effect of rise and fall of the water table. Large U isotopic changes occur with time reflecting mixing and processes of U release and reduction.

2.5.5 Vadose zone-aquifer interactions laboratory study. Important field observations including seasonal variations in CO_2, O_2, NO_3, and U concentrations are indicative of complex biogeochemical transformations generated through vadose zone-groundwater interactions. These coupled water saturation- and temperature-dependent effects arise from seasonal water table and temperature profile, yet are difficult to quantitatively explain based on sparse field measurements. To fill this gap, we will experimentally simulating deep vadose zone-groundwater interactions in the laboratory in order to obtain needed spatial and temporal resolution of hydraulic and biogeochemical processes. Two 2.00 m tall columns have been constructed to allow controlled water table fluctuations and time-dependent temperature profiles, monitoring/sampling of pore water, gas, and sediment profiles. Engagement of the broader SFA team for microbiological analyses and biogeochemical modeling will help relate laboratory results to field observations.

2.5.6 Meteoro-hydrological statistical modeling. A comprehensive statistical analysis of historical time series meteorological data (1985-2015) for the Rifle site was performed using the R software packages: hydroTSM, hydrostats, EcoHydRology, precintcon, evd, SPEI, and extRemes. We calculated a suite of hydrologic indices for daily time series precipitation data, taking into account the snowmelt, including the statistics of extreme rainfall events, high rainfall spells (magnitude, frequency, and duration), and the Standardized Precipitation Index (SPI). We calculated the potential/reference evapotranspiration, using the temperature-based and radiation-based models. Using a modified Budyko model, we estimated the actual evapotranspiration, and then calculated monthly and annual net infiltration. Calculated net infiltration showed a good agreement with estimates of the groundwater recharge rate from radioisotopic measurements. We determined that annual net infiltration percentage of precipitation varies from 4.7% to ~17.7%, with a mean of ~10%. The rainfall and evapotranspiration data were also used to calculate the multi-time-scalar Standardized Precipitation-Evapotranspiration Index (SPEI). The evaluation of the SPEI showed the intermittent pattern of droughts and wetted periods, with the increase in the duration of recurrent wet periods on the 1-year scale over the past 30 years.

2.5.7 Subsurface soil temperature dynamics. During this reporting period, the thermal data collection network at Rifle was expanded by 1) installing new thermistors in the TT-04 and TT-05 (August 2014), 2) installing shallow combined temperature and matric potential sensors at TT-04, TT-05 and along the geophysical monitoring transect near TT-05, and 3) installing a preliminary shallow thermal network at East River. Data from all of these newly installed temperature monitoring devices are regularly ingested into the SFA 2.0 Database and are being analyzed as part of ongoing modeling and data analysis efforts. For example Tran et al. (submitted, 2015) have shown that including subsurface temperature data is crucial to joint inversion of resistivity tomography data (ERT), which are in turn being used to estimate infiltration dynamics in high spatiotemporal resolution. Results have greatly improved our predictive understanding of thermal properties for the Rifle Site, which are turn are crucial to our ability to model biogeochemical transformation rates (see 2.6.2).

2.5.8 Carbon isotope variations. Decreases in the □^{13}C of soil gas CO_2 correlate with increasing CO_2 concentrations and decreasing O_2 concentrations during spring/summer indicate increasing levels of microbial activity in the unsaturated zone during that time period. The largest fluctuations occur just above the water table and are strongest in TT03 and TT05, the wells closest to the Colorado River. This matches trends in the concentration and carbon isotopic compositions of groundwater dissolved inorganic carbon (DIC) suggesting a strong relationship between the two.

2.5.9 Nitrogen isotopes and nitrogen cycling in the subsurface. Large increases in N_2O concentrations in the deep vadose zone following water level rise during spring runoff are accompanied by significant shifts in the nitrogen and oxygen isotopic compositions of the N_2O suggesting a change in microbial nitrogen cycling related to the water level rise. These isotopic trends for N_2O are coupled to changing concentrations and isotopic compositions of pore water nitrate and are consistent with a shift from nitrification during baseflow conditions to denitrification during and following groundwater peaks.

2.5.10 New scientific results and identified gaps that may shift current Tracking focus. CO_2 concentration profiles identified during this reporting period are indicative of local maxima in CO_2 generation rates in the deeper vadose zone/capillary fringe. Future work will need to include activities to distinguish between microbial versus abiotic CO_2 generation, and measure OC fluxes needed to sustain elevated rates of deeper CO_2 production.

2.6 Watershed structures and controls

The goal of the 'Watershed' Component is to quantify the key controls on watershed system behavior driven by coupled ecohydrological and biogeochemical parameters using a combination of hydrological, geochemical, geophysical, and microbiological techniques. This component integrates the SFA research themes within a field context by providing the requisite data for parameterization of floodplain (Rifle, CO) and catchment (East River, CO) scale models describing nutrient fluxes into, cycling within, and export from interconnected hydrologic units. Research activities undertaken during the reporting period were performed at the Rifle and East River sites and are described below.

2.6.1 Hydrograph-linked variations in recharge, groundwater flow direction, and biogeochemistry. The pressure transducer network and associated QA/QC was expanded and improved to monitor groundwater elevations within the Rifle aquifer. Joint with Database Management and Assimilation, team members developed a means to remove anomalous data outliers from all groundwater elevation data collected to date. The seasonally averaged, site-wide groundwater flow direction was confirmed to be in a NE-SW direction, with short-lived excursions towards the W-SW accompanying increases in Colorado River discharge. Based on the new approach, bi-weekly monitoring of groundwater spanning a gradient in aquifer redox status to assess variations in geochemical constituents, water quality parameters, and microbial community structure associated with excursions in groundwater elevation and seasonal inundation of the capillary fringe. We observed vertically- and spatially-resolved changes in aqueous metals concentrations indicative of oxygen- and nitrate-dependent metal sulfide oxidation, with this data being used to constrain temporally active metabolic pathways within GEWaSC.

New approaches were also developed to quantify controls on past and future dynamics at the Rifle Site. We developed and tested a stochastic integration method to use climate projectsions and historical variations of remote discharge data to estimate the magnitude and timing of future groundwater excursions at the Rifle Site. The analysis revealed that the snowmelt-driven water table rise at the Site is expected to occur ~1 month earlier by the end of this Century. As SFA 2.0 Rifle research has already revealed the local importance of the water table rise on nitrogen and carbon cycling, such climate-driven hydrological changes may have important implications for biogeochemical cycles at the Colorado River Basin scale. We also developed and validated a new hydrogeochemical model for uranium plume persistence at the Rifle site involving groundwater interaction with upgradient Supplemental Standards areas where residual contamination by mill tailings was left in place.

2.6.2 Thermal-hydrological infiltration model development. Using time-lapse geophysical and point measurements, we quantified dynamic variations in subsurface water and heat transport through development and testing of a coupled hydrological-thermal-geophysical inversion of both field-derived and synthetic data (Ahn et al., submitted). The inversion scheme was based on a non-isothermal hydrological model and simultaneously provided soil moisture and temperature data with a high spatiotemporal resolution, with the model explicitly considering the influence of these two variables on soil electrical conductivity. The model results indicate that temporal variations in moisture content mostly occur within the fill layer due its high water-holding capacity and overall low rainfall in the area. In contrast, moisture content changes within the underlying alluvium are minimal. Both fill and alluvium layers have high heat conductivity values, permitting seasonal variations in air temperature to propagate rapidly from land surface downward. The developed capability will allow for the detailed estimation of thermal and moisture processes using fine-scale electrical resistance tomography at Rifle and East River Sites.

2.6.3 Naturally reduced zone delineation and model parameterization. An innovative methodology was developed for the probabilistic mapping of naturally reduced zones (NRZs) within the Rifle aquifer using the induced polarization geophysical imaging conditioned by lithological data and validated by newly drilled wells (Wainwright et al., submitted). The developed approach enabled delineation of the NRZ biogeofacies type as well as the site-wide vertical distribution of the three primary lithological units controlling fluid transport (silt-rich fill, alluvium, Wasatch Formation). Both the NRZ and lithological distributions obtained from the estimation have been successful used to parameterize a three dimensional reactive transport model of the Rifle aquifer and to impose a first order constraint on the location of regions where oxygen consumption is greatest.

2.6.4 Capillary fringe nitrogen cycling. Pore water samples from suction lysimeters spanning a gradient in sediment-associated organic matter were used to document temporal variations in dissolved and gaseous nitrogen species associated with groundwater flux within the capillary fringe at Rifle. Locations having elevated organic matter and the presence of visibly reduced sediments (NRZs) showed higher absolute nitrate concentrations (4-6mM) relative to non-NRZ locations. The analysis suggested that removal of 50-90% of peak nitrate concentrations at locations within the capillary fringe coincided with inundation by groundwater during peak river discharge and resulted in increased N_2O production. Depth-dependent variations in the fractionation of ^{15}N- and $^{18}O\text{-}NO_3^-$ in residual pore water nitrate reflected variations in the mechanism of nitrate reduction (e.g. periplasmic vs. intracellular nitrate reductases, a combination of denitrification and nitrogen loss from chemolithotrophic bacteria and dominance of one over the other) and/or competing processes, such as nitrification, that complicate the residual $\delta^{15}N$ and $\delta^{18}O$ values.

2.6.5 East River catchment hydrogeochemistry Analysis of stream water and groundwater from locations throughout the East River catchment show a strong dependence upon river discharge and timing of the hydrograph excursion. Two successive rising limb phases have revealed large increases in dissolved organic carbon (DOC; 200-250µM) within the East River tied to the initial phase of snow melt, infiltration, and discharge to the river albeit prior to peak flow; stream water sulfate concentrations are negatively correlated with discharge over the entirety of the water year. Monsoonal rainfall in summer and fall corresponds to episodic increases in DOC, n δ nitrate, and chloride concentrations. Regression analysis of stream water and precipitation (rain and snow) $^{18}O\text{-}H_2O$ values indicates a mean catchment residence time of 100 days. Strong differences in groundwater geochemical composition relative to stream waters reflect the importance of hyporheic flow and microbial processing of key elements, such as carbon, nitrogen, sulfur, iron, and manganese within floodplain sediments. As at Rifle, rapid excursions in groundwater elevation accompany variations in East River discharge resulting in the existence of a capillary fringe.

2.6.6 East River vegetation-dependent soil/sediment analysis. Surface-based geophysical measurements were made within different components of the East River catchment to determine soil/sediment thickness and depth to bedrock as a function of hydrologic regime (high, medium, low energy portions of the watershed) and dominant vegetation type (spruce/fir, aspen, grass, shrub, and willow). Direct measurement of soil moisture content and temperature within a subset of these components is ongoing through deployment of autonomous data loggers to assess variations in their contribution to water flow. Soil and subsurface sediment samples recovered from spruce/fir, aspen, and meadow hillslopes, as well as the East River floodplain were analyzed for soil phase carbon content, labile dissolved organic carbon, soil pH and moisture content. Owing to the contribution of leaf litter spruce/fir and aspen covered soils had the greatest concentrations of solid phase and water-extractable organic carbon; soil pH was also significantly lower for spruce/fir-covered soils. Variations in total inorganic and organic carbon and extractable DOC were observed for floodplain soils of differing age. Older soil profiles and their longer development led to enrichment in TOC but loss of the most labile DOC fraction.

2.6.7 New scientific results or identified gaps that may shift current Watershed research focus. Development of a new hydrogeochemical model for uranium plume persistence at the Rifle site represents a paradigm shift for the site and may have broad applicability to other former mill sites within the upper Colorado River Basin (UCRB). Our demonstrated ability to link historic records of river discharge at gaging stations co-located with former mill sites with past, current, and predicted groundwater elevations in the future suggests an important future opportunity within the SFA to link climate-induced changes in hydrology at the scale of the UCRB with sites of interest to DOE and other public stakeholders.

2.7 Data Management and Assimilation (DMA)

The Data Management and Assimilation (DMA) team is building a software ecosystem to enable data synthesis and analyses across the diverse datasets and science disciplines covered by the Sustainable Systems SFA. The DMA team has very effectively supported program objectives as described below.

2.7.1 SFA 2.0 Dashboard and Broker development. The DM team has developed a data broker to connect two different external databases (RifleDB and ggkbase). Data are retrieved from the databases via web services provided by the data provider, and presented in an integrated manner via a newly developed data broker. The broker's user interface (called the SFA data dashboard) allows users to search for, visualize and download the integrated data (Fig. 12). There have been two releases and three major demonstrations of the data broker & dashboard in the last 9 months including 1) an initial demonstration at the October 2014 SFA retreat, showing the connection to the RifleDB database that hosts hydrological, geochemical and meteorological data for the Rifle site, 2) a demonstration of the beta release of the data dashboard user interface at Fall 2014 AGU Meeting, and 3) a demonstration of the broker connecting to another database - ggkbase - with metagenomic data, to program managers at the DOE BER PI Meeting in April 2015. In early June 2015, we provided a major update to the system, involving the release of the database containing over 250,000 geochemical data points alone and more than 1 million data points overall.

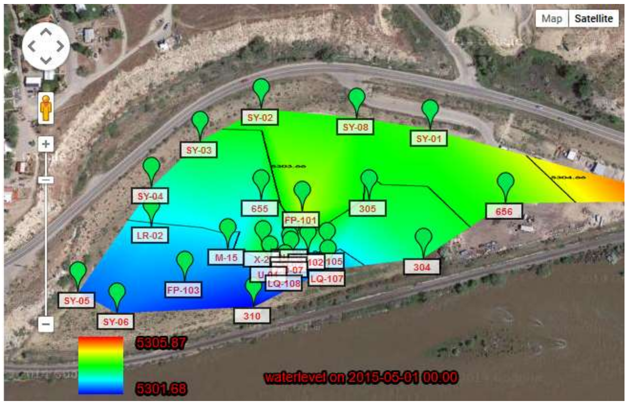


Figure 12. Visualization of water level at the Rifle Site

2.7.2 Data management, QA/QC and curation. The team has developed automated quality assurance (QA) and quality control (QC) methods to detect and identify the errors made in the process of recording, manipulating, formatting, transmitting and archiving data, or malfunctioning of sensors. The focus was on developing and implementing basic QA/QC for the DOE LM installed SOARS network that collects data from the water-level pressure transducers, vadose zone and groundwater thermistors, as well as the onsite meteorological stations. We implemented the standards developed by EPA, USGS, and Global Climate Observing System (GCOS) Climate Monitoring Principles (WMO, 2002), taking into account the specific environmental conditions and types of observations at the Rifle site.

Several additional QA/QC tasks were undertaken during this reporting period. We developed and implemented initial QA/QC procedures to identify the sources of errors (i.e, bad data) and performed cleaning up (using data filtering) of water-level time series data. Based on the analysis of field water-level data, we provided recommendations on the reinstallation and calibration of pressure transducers installed in monitoring wells. Based on the results of a recent site resurvey, prompted by data quality issues observed by the data management team, we updated the water-level database. We also developed a QC method was developed to identify and flag the erroneous temperature data lying outside of the reasonable range, as well as the occurrence of anomalous spikes (due to perturbations during water sampling events from monitoring wells). In support of the QC of the geochemical database, we identified the ranges of the concentrations and developed an approach of flagging the samples based on the evaluation ionic balance of water samples.

2.7.3 SFA 2.0 Data Management and Assimilation System Architecture

The development of the second site data package system and the expansion of the data package system to handle the submission of data associated with a paper are underway. We expect to be on track to release the first beta of these capabilities in September. The full second site database deliverable may be delayed beyond September depending on the availability of data from the second site. Data samples from each of the laboratories doing analysis of samples from the Rifle site have been collected and a new data reporting format that includes needed metadata in the reporting system has been proposed to the laboratory scientists. The new protocol is being implemented.

2.7.4_Development of as-needed data products in support of specific SFA 2.0 team emerging needs.

One of the key tasks for the DMA team was to develop the data products on demand of the SFA components scientists. These efforts included generating data files in specific formats for use in modeling codes, generating custom displays of data in response to user questions. Two examples of this are abilities (implemented on the Rifle website) for temperature depth profile visualization and data contouring. The latter, shown in Figure C, allows users to quickly assess water-level data quality in an interactive manner. This data contouring ability uses a VisIt code developed under ASCEM funding on the server side.

3.0 COLLABORATION

In addition to building on the collaborations reported in the previous annual report, new collaborations were developed in order to facilitate achievement of SFA 2.0 goals. One example of a new collaboration is a recently awarded DOE Visiting Faculty Program (VFP) to Dr. Heidi Stelzer Associate Professor of Biology at Ft. Lewis College in Durango, CO. Dr .Stelzer will focus on coupled phenological-hydrological behavior within the Harte et al. warming meadow experimental plots — to be done in conjunction with the to-be-submitted Banfield-led DOE-JGI CSP proposal "Genome-resolved metagenomic analysis of metabolic potential at the watershed scale”. The goal will be to link this data to several decades of natural (i.e., non-experimentally impacted) phenological data collected by Dr. David Inouye within the East River Catchment. This collaboration is an exceptional opportunity to link vegetation and subsurface biogeochemistry in a way that has not previously been possible. Other key new collaborations include a third round of terrabase-level sequencing awarded by the Joint Genome Institute to Jill Banfield for sequencing of East River samples. We also have a very significant new collaboration with the Interoperable Design of Extreme-scale Application Software (IDEAS) Project in which East River is one of the main use cases for development of integrated modeling codes (see https://ideas-productivity.org/).Another example is a successful proposal for use of the SGM beamline at the Canadian Light Source (CLS). The beam time has been awarded for December 2015 for studying single organic carbon molecules. The work is being conducted in collaboration with CLS scientists Dr. Adam Gillespie and Dr. Tom Reiger and represents a new, productive collaboration for the SFA. Kate Maher (Stanford) has also recently been awarded a BER grant for research at the East River, which will be performed in collaboration with the SFA 2.0.

4.0 PRODUCTIVITY, COLLABORATION, OUTREACH

A complete description of SFA 2.0 products is provided in the Appendix, including journal publications, outreach, community service, invited presentations, and abstracts. The Appendix also provides information about other relevant activity or recognition, such as workshops or special session organization, awards, and leadership positions. In summary, since our last progress report (2014) this project published 23 journal publications and 7 invited talks Of the 23 papers, 11 were published in journals with an impact factor > 5.

Appendix I. SFA 2.0 Products List:

Publications (Motivated and Supported by SFA 2.0) Published and in Press

Journal Title	2014/5-Year Impact Factor (Ranked)	Total Articles
Genome Research	15.567	1
Nature Communications	11.904	1
Current Biology	10.134	1
ISME Journal	9.438	2
Advances in Agronomy	6.758	1
Environmental Science & Technology	6.326	3
Environmental Microbiology	6.312	2
Geochimica et Cosmochimica Acta	4.933	2
Water Resources Research	4.144	1
Journal of Environmental Quality	2.972	1
Colloids and Surfaces A-Physicochemical and Engineering Aspects	2.832	1
Computational Geosciences	1.883	6
Procedia Earth and Planetary Science	1.088 (SNIP)	1
Total		**23**

PUBLICATIONS

2015

1. Beisman, J., R. Maxwell, A. Navarre-Sitchler, C. Steefel, and S. Molins (2015), ParCrunchFlow: an efficient, parallel reactive transport simulation tool for physically and chemically heterogeneous saturated subsurface environments, Computat Geosci, 19(2), 403-422, doi:10.1007/s10596-015-9475-x.
2. Binley, A., S. S. Hubbard, J. A. Huisman, A. Revil, D. A. Robinson, K. Singha, and L. D. Slater (2015), The emergence of hydrogeophysics for improved understanding of subsurface processes over multiple scales, Water Resour Res, n/a-n/a, doi:10.1002/2015WR017016.
3. Castelle, C. J., K. C. Wrighton, B. C. Thomas, L. A. Hug, C. T. Brown, M. J. Wilkins, K. R. Frischkorn, S. G. Tringe, A. Singh, L. M. Markillie, R. C. Taylor, K. H. Williams, and J. F. Banfield (2015), Genomic Expansion of Domain Archaea Highlights Roles for Organisms from New Phyla in Anaerobic Carbon Cycling, *Curr Biol*, *25*(6), 690-701, doi:10.1016/j.cub.2015.01.014.
4. Handley, K. M., K. C. Wrighton, C. S. Miller, M. J. Wilkins, R. S. Kantor, B. C. Thomas, K. H. Williams, J. A. Gilbert, P. E. Long, and J. F. Banfield (2015), Disturbed subsurface microbial communities follow equivalent trajectories despite different structural starting points, *Environ Microbiol*, *17*(3), 622-636, doi:10.1111/1462-2920.12467.
5. Holmes, D. E., L. Giloteaux, A. K. Chaurasia, K. H. Williams, B. Luef, M. J. Wilkins, K. C. Wrighton, C. A. Thompson, L. R. Comolli, and D. R. Lovley (2015), Evidence of Geobacter-associated phage in a uranium-contaminated aquifer, *ISME J*, *9*(2), 333-346, doi:10.1038/ismej.2014.128.
6. Hug, L. A., B. C. Thomas, C. T. Brown, K. R. Frischkorn, K. H. Williams, S. G. Tringe, and J. F. Banfield (2015), Aquifer environment selects for microbial species cohorts in sediment and groundwater, *ISME J*, doi:10.1038/ismej.2015.2.
7. Hug, L. A., B. C. Thomas, I. Sharon, C. T. Brown, R. Sharma, R. L. Hettich, M. J. Wilkins, K. H. Williams, A. Singh, and J. F. Banfield (2015), Critical biogeochemical functions in the subsurface are associated with bacteria from new phyla and little studied lineages, *Environ Microbiol*, doi:10.1111/1462-2920.12930.
8. Kleber, M., K. Eusterhues, M. Keiluweit, C. Mikutta, R. Mikutta, and P. S. Nico (2015), Mineral–Organic Associations: Formation, Properties, and Relevance in Soil Environments, in *Advances in Agronomy*, edited by D. L. Sparks, pp. 1-140, Elsevier Inc., Academic Press.
9. Long, P. E., K. H. Williams, J. A. Davis, P. M. Fox, M. J. Wilkins, S. B. Yabusaki, Y. Fang, S. R. Waichler, E. S. F. Berman, M. Gupta, D. P. Chandler, C. Murray, A. D. Peacock, L. Giloteaux, K. M. Handley, D. R. Lovley, and J. F. Banfield (2015), Bicarbonate impact on U(VI) bioreduction in a shallow alluvial aquifer, *Geochim Cosmochim Acta*, *150*(0), 106-124, doi:10.1016/j.gca.2014.11.013.
10. Luef, B., K. R. Frischkorn, K. C. Wrighton, H. Y. N. Holman, G. Birarda, B. C. Thomas, A. Singh, K. H. Williams, C. E. Siegerist, S. G. Tringe, K. H. Downing, L. R. Comolli, and J. F. Banfield (2015), Diverse uncultivated ultra-small bacterial cells in groundwater, *Nat Commun*, *6*, doi:10.1038/ncomms7372.
11. Mayer, K. U., P. Alt-Epping, D. Jacques, B. Arora, and C. Steefel (2015), Benchmark problems for reactive transport modeling of the generation and attenuation of acid rock drainage, *Computat Geosci*, 1-13, doi:10.1007/s10596-015-9476-9.
12. Sharon, I., M. Kertesz, L. A. Hug, D. Pushkarev, T. A. Blauwkamp, C. J. Castelle, M. Amirebrahimi, B. C. Thomas, D. Burstein, S. G. Tringe, K. H. Williams, and J. F. Banfield (2015), Accurate, multi-kb reads resolve complex populations and detect rare microorganisms, *Genome Res*, *25*(4), 534-543, doi:10.1101/gr.183012.114.
13. Varadharajan, C., R. Y. Han, H. R. Beller, L. Yang, M. A. Marcus, M. Michel, and P. S. Nico (2015), Characterization of Chromium Bioremediation Products in Flow-Through Column Sediments Using Micro-X-ray Fluorescence and X-ray Absorption Spectroscopy, *J Environ Qual*, *44*(3), 729-738, doi:10.2134/jeq2014.08.0329.

2014

14. Alessi, D. S., J. S. Lezama-Pacheco, N. Janot, E. I. Suvorova, J. M. Cerrato, D. E. Giammar, J. A. Davis, P. M. Fox, K. H. Williams, P. E. Long, K. M. Handley, R. Bernier-Latmani, and J. R. Bargar (2014), Speciation and Reactivity of Uranium Products Formed during in Situ Bioremediation in a Shallow Alluvial Aquifer, *Environ Sci Technol*, *48*(21), 12842-12850, doi:10.1021/es502701u.
15. Arora, B., S. S. Şengör, N. Spycher, and C. Steefel (2014), A reactive transport benchmark on heavy metal cycling in lake sediments, *Computat Geosci*, 1-21, doi:10.1007/s10596-014-9445-8.
16. Babchin, A. J., and B. Faybishenko (2014), On the capillary pressure function in porous media based on relative permeabilities of two immiscible fluids, *Colloid Surface A*, *462*, 225-230, doi:10.1016/j.colsurfa.2014.09.005.
17. Beller, H. R., L. Yang, C. Varadharajan, R. Y. Han, H. C. Lim, U. Karaoz, S. Molins, M. A. Marcus, E. L. Brodie, C. I. Steefel, and P. S. Nico (2014), Divergent Aquifer Biogeochemical Systems Converge on Similar and Unexpected Cr(VI) Reduction Products, *Environ Sci Technol*, *48*(18), 10699-10706, doi:10.1021/es5016982.
18. Druhan, J. L., M. Bill, H. Lim, C. Wu, M. E. Conrad, K. H. Williams, D. J. DePaolo, and E. L. Brodie (2014), A large column analog experiment of stable isotope variations during reactive transport: II. Carbon mass balance, microbial community structure and predation, *Geochim Cosmochim Ac*, *124*, 394-409, doi:10.1016/j.gca.2013.08.036.
19. Molins, S., J. Greskowiak, C. Wanner, and K. U. Mayer (2014), A benchmark for microbially mediated chromium reduction under denitrifying conditions in a biostimulation column experiment, *Computat Geosci*, 1-18, doi:10.1007/s10596-014-9432-0.
20. Steefel, C. I., C. A. J. Appelo, B. Arora, D. Jacques, T. Kalbacher, O. Kolditz, V. Lagneau, P. C. Lichtner, K. U. Mayer, J. C. L. Meeussen, S. Molins, D. Moulton, H. Shao, J. Šimůnek, N. Spycher, S. B. Yabusaki, and G. T. Yeh (2014), Reactive transport codes for subsurface environmental simulation, *Computat Geosci*, 1-34, doi:10.1007/s10596-014-9443-x.
21. Steefel, C. I., J. L. Druhan, and K. Maher (2014), Modeling Coupled Chemical and Isotopic Equilibration Rates, *Procedia Earth and Planetary Science*, *10*(0), 208-217, doi:10.1016/j.proeps.2014.08.022.
22. Stucker, V. K., D. R. Silverman, K. H. Williams, J. O. Sharp, and J. F. Ranville (2014), Thioarsenic Species Associated with Increased Arsenic Release during Biostimulated Subsurface Sulfate Reduction, *Environ Sci Technol*, *48*(22), 13367-13375, doi:10.1021/es5035206.
23. Wanner, C., J. Druhan, R. Amos, P. Alt-Epping, and C. Steefel (2014), Benchmarking the simulation of Cr isotope fractionation, *Computat Geosci*, 1-25, doi:10.1007/s10596-014-9436-9.

Outreach, DOE & Community Service, Awards/Recognition

- Phil Long and Ken Williams gave a talk on SFA 2.0 at the Rifle City Council Meeting
- ESS 2015 PI meeting Session Lead Roles (Hubbard, Williams))
- Virtual ecosystem report (Steefel, Brodie)
- Complex Soils Systems Conference – September, 2014
  Fall AGU Booth, San Francisco, 2014. 'Genomes-to-Watershed' Day
- Rifle City Council Meeting – June 2014
- SFA 2.0 Fall 2014 e-Newsletter
- SFA 2.0 Video Playlist

Leadership and Editorship Positions

- Beller, H.R. - Associate Editor, BMC Biotechnology
- Beller, H.R. - Editorial Board, Environmental Science & Technology
- Brodie, E. – Editorial Board, Microbiome
- Brodie, E. – Academic Editorial Board, PeerJ
- Brodie, E. – Associate Editor, Frontiers in Microbiology

- Faybishenko, B., Co-Editor, AGU/Wiley monograph "Dynamics of Fluids and Transport in Fractured Porous Media"
- Faybishenko, B. – Co-Editor, AGU/Wiley monograph "Dynamics of Fluids and Transport in Fractured Porous Media"
- Faybishenko, B. – Senior Editor (Environmental Science) of the Oxford Research Encyclopedia
- Holman, H. - Editorial Board, Biomedical Spectroscopy and Imaging
- Holman, H. - Exemplar-Zero (E-Z) Initiative Core Advisory Council
- Holman, H. - International Scientific Advisory, HUMANITAD
- Hubbard, S.S., Associate Director Berkeley Water Center
- Hubbard, S.S., DOE BER Advisory Board (BERAC)
- Hubbard, S.S., Associate Editor, JGR-Biosciences
- Hubbard, S.S., ASCEM Sr. Advisor
- Hubbard, S.S., Helmoltz Assn. Terrestrial Advisory Committee
- Hubbard, S.S., Clemson-USC DOE EPSCoR Advisory Board
- Steefel, C. - Associate Editor, Geochimica et Cosmochimica
- Steefel, C. - Associate Editor, Journal of Contaminant Hydrology
- Tokunaga, T. - Associate Editor, Water Resources Research
- Tokunaga, T. - Associate Editor Vadose Zone Journal
- Williams, K. - Associate Editor, JGR-Biogeosciences

Awards:

- J. Banfield, Elected to the Australian Academy of Science as a corresponding member (only two people are elected in this category each year).
- J. Banfield, Honorary doctorate, ETH, Switzerland
- J. Banfield, Honorary doctorate, Ben Gurion University, Israel
- S. Hubbard, 2014 member of the University of California, Berkeley Civil and Environmental Engineering (CEE) Department academy of Distinguished Alumni.
- S. Hubbard, Distinguished technical communication 2013-2014 award for the 'BER Virtual Laboratory: Innovative Framework for Biological and Environmental Grand Challenges', DOE/SC-0156, bestowed by the Society for Technical Communication, Washington DC

Invited/Keynote Presentations (partial list)

- J. Banfield, "The diversity and possible subsurface biogeochemical roles of enigmatic bacteria and archaea from massive candidate phyla radiations" 2015 ESS PI Meeting
- P.E. Long, predictive understanding of subsurface biogeochemical functioning: using genomes to inform watershed-scale models." GSA 2014
- B. Faybishenko, "Depth- and time-resolved temperature of the vadose zone and a shallow alluvial aquifer beneath a Colorado River floodplain." GSA 2014
- J. Banfield, "prediction of the Biogeochemical Roles of Uncultivated Bacteria and Archaea in the Subsurface." Goldschmidt 2014
- K.H. Williams, "A Floodplain Perspective on Elemental Cycling and Uranium Plume Persistence." Goldschmidt 2014
- C.I. Steefel, "The GEWaSC Framework: Multiscale Modeling of Coupled Biogeochemical, Microbiological, and Hydrological Processes" Goldschmidt 2014
- C. Cismasu, "Iron and Carbon Dynamics during the Reductive Transformation of Organic Matter-Rich FE (III)" Goldschmidt 2014

Abstracts (SFA and SFA-supported); Partial List

1. Goldschmidt 2014 – SFA 2.0 Abstract book
2. AGU Fall 2014 – SFA Abstract Book
3. Arora, B.,Spycher, N., Molins, S., Steefel, C.I., B31B-0019: Modeling the biogeochemical response of a floodplain aquifer impacted by seasonal temperature and water table variations, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
4. Bargar, J., Janot, N., Jones, M.E., Bones, S.E., Lezama-Pacheco, J., Fendorf, S.E., Long, P.E., Williams, K.H., Bush, R.P., B21B-0040: Importance of organic matter-uranium biogeochemistry to uranium plume persistence in the Upper Colorado River Basin, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
5. Beller, H. R., P. Zhou, T. C. Legler, A. Chakicherla, P. A. O'Day. 2014. Genome-enabled studies of anaerobic, nitrate-dependent iron oxidation in Thiobacillus denitrificans. Poster at the 114th General Meeting of the American Society for Microbiology, Boston, MA, May 2014.
6. Beller, H.R., Jewell, T.N., Karaoz, U., Thomas, B.C., Banfield, J.F., Brodie, E., Williams, K.H., B22D-08: Metatranscriptomic evidence of chemolithoautotrophy in the Rifle (CO) subsurface relevant to C, S, N, and Fe cycling, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
7. Bill, M., Conrad, M.E., Kolding, S., Williams, K.H., Tokunaga, T.K., B23B-0203: Seasonal variations and cycling of nitrous oxide using nitrogen isotopes and concentrations from an unsaturated zone of a floodplain, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
8. Brodie, E., King, E., Molins, S., Karaoz, U., Johnson, J.N., Bouskill, N., Hug, L.A., Thomas, B.C., Castelle, C.J., Beller, H.R., Banfield, J.F., Steefel, C.I., B42B-05: Beyond the blueprint: development of genome-informed trait-based models for prediction of microbial dynamics and biogeochemical rates, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
9. Chen, J., Hubbard, S.S., and Williams, K.H., B31B-0022: Estimating groundwater dynamics at a Colorado floodplain site using historical hydrological data and climate information, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
10. Christensen, J.N., Shiel, A.E., Conrad, M.E., Williams, K.H., Dong, W., Tokunaga, T.K., Wan, J., Long, P.E., and Hubbard, S.S., H43N-1174: Uranium and Strontium Isotopic Study of the Hydrology of the Alluvial Aquifer at the Rifle Former U Mine Tailings Site, Colorado, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
11. Conrad, M., Arora, B., Williams, K.H., Bill, M., Spycher, N., Steefel, C.I., Tokunaga, T.K., and Hubbard, S.S., B31B-0016: Using Concentrations and Isotopic Compositions of CO2 to Distinguish Microbial Production of CO2 in Unsaturated Zone Sediments in Hydrogeochemical Models, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
12. Dong, W., Wan, J., Tokunaga, T.K., Gilbert, B., Kim, Y., Williams, K.H., 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, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
13. Druhan, J., Bill, M., Lim, H.C., Wu, C., Conrad, M.E., Williams, K.H., DePaolo, D.J., Brodie, E., B42B-02: Evidence of a dynamic microbial community structure and predation through combined microbiological and stable isotope characterization, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
14. Farrington, S., Van Wyck, N.E., Williams, K.H., H13C-1131: Development of a sensor for measuring in situ soil moisture in continuous spatial profile, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
15. Hubbard, S.S. and Arora, B. (Chairs), B33B: Characterizing Spatial and Temporal Variability of Hydrological and Biogeochemical Processes Across Scales I Posters, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.

16. Hubbard, S.S., Agarwal, D., Banfield, J.F., Beller, H.R., Brodie, E., Long, P., Nico, P.S., Steefel, C.I., Tokunaga1, T.K., Williams, K.H., and the Sustainable Systems SFA 2.0 Team, B31B-0020: Genome-to-Watershed Predictive Understanding of Terrestrial Environments, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
17. Jewel T., Karaoz, U., Thomas, B.C., Banfield, J.F., Brodie, E., Williams, K.H., Beller, H.R., B11H-0153: Metatranscriptomic analysis of groundwater reveals an active anammox bacterial population, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
18. Kenwell, A.M., Navarre-Sitchler, A., Prugue, R., Spear, J.R., Williams, K.H., Maxwell, R.M., B33B-0166: Using geochemical indicators to distinguish high biogeochemical activity in sediments, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
19. King, E., Molins, S., Karaoz, U., Johnson, J.N., Bouskill, N., Hug, L.A., Thomas, B.C., Castelle, C.J., Beller, H.R., Banfield, J.F., Steefel, C.I., Brodie, E., B31B-0021: Modeling microbial biogeochemistry from terrestrial to aquatic ecosystems using trait-based approaches, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
20. Long, P.E., Faybishenko, B., Williams, K.H., Potter, B., Versteeg, R.J., Yabusaki, S.B., Tokunaga, T.K., Depth- and time-resolved temperature of the vadose zone and a shallow alluvial aquifer beneath a Colorado River floodplain, 2014 GSA Annual Meeting, Vancouver, BC, 19-22 October 2014.
21. Long, P.E., Hubbard, S.S., Banfield, J., Beller, H, Brodie, E., Nico, P.S., Steefel, C., Tokunaga, T.K., Williams, K.H., Agarwal, D., Predictive understanding of subsurface biogeochemical functioning: using genomes to inform watershed-scale models, 2014 GSA Annual Meeting, Vancouver, BC, 19-22 October 2014.
22. Madrid, V.M., M. Singleton, B.K. Esser, and H.R. Beller. 2014. An Interdisciplinary Monitored Natural Attenuation Study of Groundwater Nitrate at a High-Explosive Test Facility in California. Poster at the 9th International Conference on Remediation of Chlorinated and Recalcitrant Compounds, Monterey, CA, May, 2014.
23. Nico, P.S., Hess, N.J., Tang, J., (Chairs) B31L: Soil Organic Matter Dynamics: Novel Techniques, Big Data, and Functional Models III, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
24. O'Day, P. A., J. Chorover, C. Steefel, H. R. Beller, M. Kanematsu, N. Perdrial, E. Reinoso-Maset, A. Vazquez-Ortega. 2014. Scaling of molecular processes to quantify biogeochemical reaction and transport of uranium in subsurface systems. Oral presentation at the 2014 TES SBR PI Meeting, Potomac, MD, May, 2014.
25. Pan, D., Williams, K.H., Robbins, M., Webber, K.A., B21B-0039: Redox fluctuation influences viral abundance in the reduced zone of a shallow alluvial aquifer in Rifle, CO, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
26. Pribulick, C., Maxwell, R.M., Williams, K.H., Carroll, R.W.H., H31H-0720: A high resolution, integrated approach to modeling climate change impacts to a mountain headwaters catchment using ParFlow, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
27. Stucker, V., Ranville, J.F., Williams, K.H., Conveners, Session on Contaminant biogeochemical cycles and elemental speciation: implications for remediation of subsurface environments I American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
28. Stucker, V., Ranville, J.F., Williams, K.H., Conveners, Session on Contaminant biogeochemical cycles and elemental speciation: implications for remediation of subsurface environments II Posters Session, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
29. Tokunaga, T.K., Wan, J., Dong, W., Kim, Y., Williams, K.H., Conrad, M.E., Christensen, J.N., Bill, M., Faybishenko, B., Hobson, C., Dayvault, R., Long, P.E., and Hubbard, S.S., 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, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
30. Tran, A.P., Dafflon, B., Hubbard, S.S., Kowalsky, M.B., Tokunaga, T.K., Faybishenko, B., and Long, P.E., H54B-06: Monitoring Soil Hydraulic and Thermal Properties using Coupled Inversion of Time-

lapse Temperature and Electrical Resistance Data, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.

31. Wainwright, H., Hubbard, S.S., Arora, B., (Chairs) B44B:Characterizing spatial and temporal variability of hydrological and biogeochemical processes across scales II, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
32. Wan,J., Dong, W., Kim, Y., Tokunaga, T.K., Bill, M., Conrad,M.E., Williams,K.H., Long, P.E., and Hubbard, S.S., B33B-0164: Subsurface Carbon Cycling Below the Root Zone, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
33. Williams, K.H., Bucker, M., Flores Orozco, A., Hobson, C., Robbins, M., B33B-0163: Novel approaches for delineating and studying “hotspots” and “hot moments” in fluvial environments, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.
34. Zaunbrecher, L.K., Elliott, W.C.., Lim, D., Pickering, R.A., Williams, K.H., Long, P.E., Qafoku, N.P., B21B-0043: Clay mineralogy of soils and sediments from an alluvial aquifer, Rifle, Colorado, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014.