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Pacific Northwest National Laboratory SFA Annual Report

Influences of Hydrologic Exchange Flows on River Corridor and Watershed Biogeochemical Function

June 2018

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PNNL SBR Scientific Focus Area Annual Report FY2018

**Influences of Hydrologic Exchange Flows on River Corridor and Watershed
Biogeochemical Function**

2018 Annual Report
June 30, 2018

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I. PROGRAM OVERVIEW

The Pacific Northwest National Laboratory (PNNL) Subsurface Biogeochemical Research (SBR) Science Focus Area (SFA) is transforming fundamental understanding of the hydrobiogeochemical function of dynamic river corridor ecosystems and is using this new knowledge to develop a predictive watershed modeling framework encapsulating river corridor processes.

We are studying the interactions among variable river surface elevation (“stage”), hydromorphic setting, and hydrogeologic heterogeneity and determining how those interactions influence river corridor hydrobiogeochemical function. Our approach builds from a foundation in understanding fundamental processes to reveal their cumulative effects on watershed-scale hydrobiogeochemical function. The pivotal linkages between these elements are hydrologic exchange flows (HEFs), the dynamic exchange of water and chemical constituents between river channels and adjacent subsurface environments that comprise the river corridor (Harvey and Gooseff, 2015). HEFs are a vital aspect of watershed function that are poorly represented in system-scale models. We are evaluating mechanistic linkages between variable river stage and HEFs and revealing those processes governing the biogeochemical influences of hydrologic history and the character (e.g., thermodynamic properties) of organic carbon. Using the resulting knowledge of governing processes, we are developing and extending community models that can be used to predict hydrobiogeochemical function in managed and unmanaged systems across a broad range of environmental conditions.

Our long-term objective is to mechanistically link large scale drivers of change (e.g., changing climate and land use) with features of managed energy-water systems (e.g., hydroelectric dams) that modulate the influences of these drivers on HEFs and their biogeochemical consequences. Our approach is based on translation of fundamental process understanding into predictive models that are applicable to other watersheds. This approach will enable inter-agency collaboration focused on solving pragmatic issues related to water quality and ecosystem health as well as providing a mechanistic foundation for representing river corridor processes in Earth system models. The long-term outcomes will be the development and use of fundamental knowledge to 1) forecast and mitigate river corridor and watershed environmental issues that impact the functioning and operation of the nation’s complex energy-water systems, and 2) reduce uncertainty in major cross-ecosystem water and nutrient fluxes.

Progress toward this objective is achieved through three integrated research campaigns (RCs). SFA team members work on multiple campaigns, campaign activities are jointly coordinated by the PI team, and high-impact publications are targeted that integrated information across the three campaigns to address high-level project objectives. The RCs are structured from a top-down perspective in keeping with the concept of iterative model-driven experimentation and observation:

- The *Systems Models* RC (Campaign A) uses numerical experimentation of linked river corridor and watershed models at multiple scales and levels of process fidelity. These models reveal the cumulative effects of small-scale governing processes (Mechanistic Models and Process Studies RCs) and their appropriate representation in larger-scale models. Systems models are constructed by generalizing outputs from the Mechanistic Models RC and are used to guide observational and experimental studies conducted by the Process Studies RC.
- The *Mechanistic Models* RC (Campaign B) is developing high-resolution mechanistic models of HEFs and associated reactive transport processes. These models are being integrated with experiments and observations (Process Studies RC) to reveal processes governing hydrobiogeochemical function within hydromorphic units. This information is used to inform development of larger-scale models of reduced complexity (reduced-order models) for the Systems Models RC.
- The *Process Studies* RC (Campaign C) performs field and laboratory data collection and experimentation guided by mechanistic and system models. These studies provide process knowledge to the two modeling RCs, enabling an iterative approach that is revealing processes underlying interactions among biogeochemical function, variable discharge, hydromorphology, and hydrogeology.

II. KEY SCIENTIFIC QUESTIONS UNDER INVESTIGATION

The vision of the PNNL SBR SFA is to develop a fundamental and comprehensive scientific understanding of the influences of hydrologic exchange flows (HEFs, Figure 1) on river corridor biogeochemical and ecological functions and to integrate this new-found scientific understanding into a first-of-kind hydrobiogeochemical model of the river corridor, linked as a critical component of watershed systems models. Accordingly, we are pursuing the resolution of fundamental scientific hypotheses designed to advance understanding of coupled hydrobiogeochemical processes. At the same time, we are developing a hierarchical multiscale modeling framework that integrates scientific understanding into a predictive watershed modeling capability with wide applicability. This new model capability will improve prediction of watershed system responses to large-scale drivers of change and enable effective management of human water and energy systems that modulate river corridor function. Our vision can be summarized in terms of scientific grand challenge and mission-relevance statements:

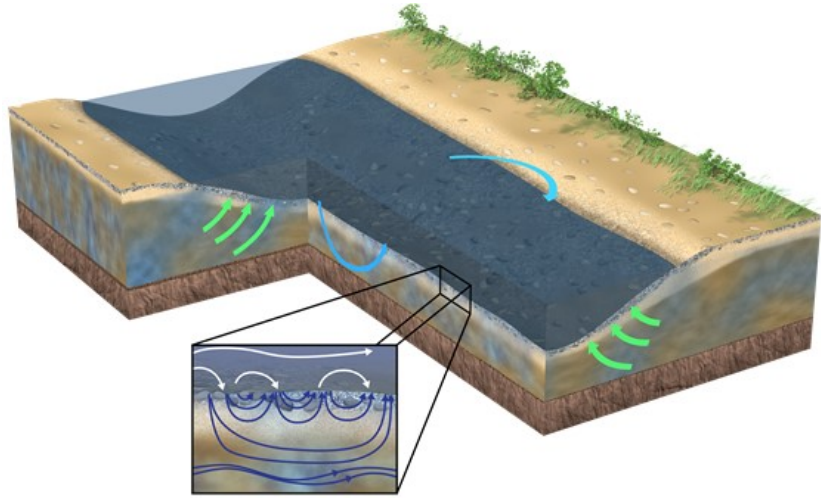


Figure 1. Schematic diagram of different types and scales of Hydrologic Exchange Flows (HEFs), including bedform-driven small-scale vertical exchange (inset) and large-scale bank exchanges driven by temporal variations in river discharge and stage.

Scientific Grand Challenge: *Develop fundamental understanding of the processes that govern influences of hydrologic exchange flows on water quality, nutrient dynamics, and ecosystem health in dynamic river corridor systems.*

Biological and Environmental Research (BER) Mission-Relevance Challenge: *Provide a mechanistic basis for predictive modeling of river corridor function, and incorporate this new understanding into community watershed modeling frameworks.*

The conceptualization of hydrologic exchanges driven by the interaction of dynamic river discharge/stage with a variety of hydromorphic and hydrogeologic structures provides the central construct for both fundamental process studies and development of a hierarchical multiscale modeling framework. This conceptualization, framed in terms of the challenges above, leads to the following high-level science questions that guide our research activities:

1. What are the hydrobiogeochemical processes that link river stage fluctuations and hydromorphic setting to distributions of hydrologic exchange fluxes, residence times, and reaction rates? *This question motivates the Scientific Grand Challenge above.*
2. How do governing processes change across scales, how do those changes govern the cumulative effects of smaller-scale processes on reach- to watershed-scale phenomena, and what is the appropriate representation of smaller-scale processes in larger-scale predictive hydrobiogeochemical models? *This question motivates the BER Mission-Relevance Challenge above.*

The resolution of these science questions will fill two critical knowledge gaps that exist in scientific understanding of river corridor and watershed hydrobiogeochemistry: 1) Poor understanding of dynamic river stage influences on biogeochemical and ecological processes and limited representation of these processes in reactive transport models, and 2) poor understanding of how hydrologic exchange processes and associated biogeochemical reactions within the river corridor impact watershed-scale biogeochemical function, and specifically how changes in large-scale drivers of river corridor environmental conditions (such as land use and climate change, hydropower operations, irrigated agriculture) impact those cumulative effects. Our research program is designed to resolve these gaps in scientific understanding, and our experimental field site is ideally suited as a natural laboratory for this research.

III. NATIONAL LABORATORY PROGRAM STRUCTURE

The PNNL SBR-SFA is led by a Principal Investigator (PI, Tim Scheibe), two Co-PIs (Xingyuan Chen and James Stegen), and a Watershed Coordinator (Maoyi Huang) (Figure 2). A Laboratory Research Manager (Charlette Geffen) provides laboratory oversight and guidance to the PI and Co-PIs, and serves as the primary point-of-contact with the DOE Office of Biological and Environmental Research (BER). We have also engaged a committee of Science Advisors who provide mentorship to the PI Team and offer their perspectives as experienced and knowledgeable observers. The SFA is organized around three Research Campaigns (RCs), each of which is led by one of the three PIs. Each RC comprises two to three major Activities; each Activity is organized into several Sub-Activities. Activity Leads are responsible for coordinating research within each Activity, and are both Key Staff and members of the SFA Leadership Team. The Watershed Coordinator coordinates SFA watershed-scale activities with those in other large-scale BER programs including E3SM, IM3, and NGEE, in which she is also an active participant, and acts as a member of the PI Team. Other Key Staff have cross-cutting responsibilities across multiple Activities or Sub-Activities, and contributing staff (including funded collaborators) are disciplinary

experts that lead or contribute to one or more Sub-Activities. SFA researchers are drawn from all four research directorates at PNNL as dictated by the interdisciplinary nature of SFA research. The RCs, Activities, and Sub-Activities have been jointly designed and are closely coordinated by the Leadership Team to accomplish overall project scientific objectives.

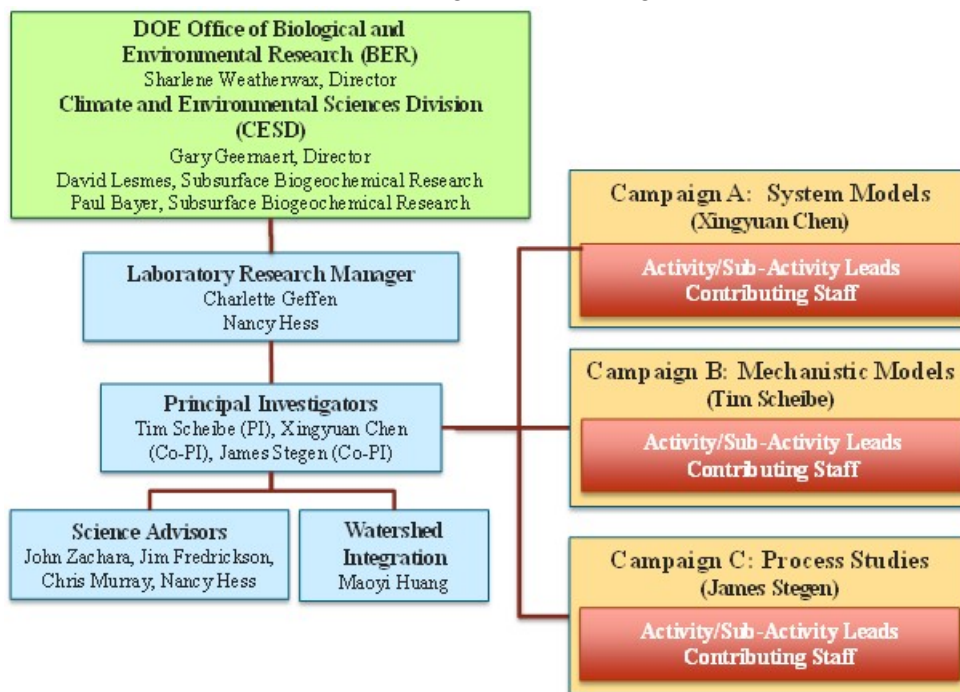


Figure 2. PNNL SBR SFA project team organizational structure.

Our management philosophy and process is characterized by 1) intentional, regular and transparent communication and documentation of progress through a number of channels, and 2) emphasis on individual awareness of and accountability to team outcomes. This, in the context of our team values of

scientific excellence, creativity, collaboration, and mentorship, leads to active engagement of the entire project team in pursuing the integrated objectives of the project. Primary avenues for team coordination and communication are: 1) regular meetings at a variety of organizational levels, and 2) extensive utilization of agile project management tools Confluence and Jira.

IV. PERFORMANCE MILESTONES AND METRICS

Review of Scientific Progress Toward Program Objectives and Milestones

Research Campaign A (RC-A): System Models

Overall Objectives: The Systems Models Campaign aims to reveal the cumulative effects of relatively small-scale governing processes on system-scale watershed function and their appropriate representation in watershed models.

- Quantify the cumulative effects of mechanistic river corridor HEFs and biogeochemistry (RC-B and RC-C) on large-scale nutrient cycling, water quality (including temperature), contaminant mobility, and land surface fluxes.
- Identify the critical scale-dependent process couplings that govern the translation of hydromorphic unit scale (features such as pools, sediment bars, and meanders on the order of hundreds of meters to kilometers) mechanistic processes to reach and watershed-scale function (e.g., water quality, ecological health, and nutrient processing). Quantify those process couplings in terms of reduced-order models applicable at system scales.
- Advance the scientific basis for river-network-scale river corridor modeling by replacing empirical formulations in current state-of-art models with mechanistically-based reduced-order models and parameterizations.
- Incorporate the new river corridor model into a prototype watershed-scale modeling framework that will have broad applicability to both scientific investigations of the cumulative effects of river corridor hydrobiogeochemistry on watershed function and applied predictions of watershed system response to environmental perturbations and human controls.

Key Contributions of this Research Campaign to the SFA: Numerical experimentation using linked models at multiple scales and levels of process fidelity, integrated with experiments and observations, can shed light on the manner in which emergent system functions arise from interactions of complex hydrobiogeochemical processes. This campaign is using this approach to assess the importance of river corridor processes in hydrologic exchange flow, heat transport, contaminant mobilization and transport, and C and N transformations and their gaseous emissions at the land surface within a river reach or watershed. The resulting knowledge will directly contribute to the resolution of Science Question 2. To enable this, we are developing a first-of-kind river-network model of HEFs and associated biogeochemical processes guided by high-resolution mechanistic model simulations at the hydromorphic unit scale (from RC-B). This new river corridor model will be coupled with other existing watershed model components to create a prototype watershed-scale modeling framework that directly accounts for river corridor hydrobiogeochemistry in predictions of watershed-scale nutrient processing, water quality, and river ecology (e.g., microbial community and riparian zone plant dynamics). A critical aspect of the coupling is implementation and testing of alternative reduced order modeling approaches to determine the appropriate level of complexity for simulating watershed scale complex system behavior. System model testing includes evaluating ability to reproduce mechanistic model predictions where available, comparing model outputs to large-scale observations such as remote sensing products and environmental monitoring data from EPA and USGS, and comparing predictions to simpler empirical models.

FY18 Research Targets

FY18 Science Plan Milestone: Initial evaluation of the influence of large-scale HEFs driven by variable stage on reach-scale biogeochemical fluxes. Incorporate multi-rate Transient Storage Models (TSMs) into the river routing module SWATR to initiate the development of the river corridor model. Collaborate with RC-B to map hydromorphic features within the Upper-Columbia Priest Rapids watershed.

Progress Brief for FY18

Activities have focused on establishing a baseline for evaluating the influence of HEFs on river corridor and watershed biogeochemical functions by initiating the reach-scale HEF modeling with mechanistic PFLOTRAN simulations and developing a river corridor module based on the existing river routing component of the Soil and Water Assessment Tool (SWATR). Key elements of progress and associated scientific findings are as follows:

Reach-scale modeling revealed spatio-temporal dynamics of HEFs of dam-regulated Hanford Reach river corridor: Existing data and groundwater models on both sides of the Hanford Reach of the Columbia River were compiled into a reach-scale model of HEFs using the PFLOTRAN code. The resulting 3D numerical simulations provided new insights into the complex spatial and temporal dynamics of HEFs from the km- to reach-scale (10s of km) along this highly regulated river corridor. Multiple numerical tracers were introduced along selected segments of the river boundary to track the contribution of river water to groundwater flow. Particle tracking was performed to reveal exchange pathways and estimate the distributions of river water residence time.

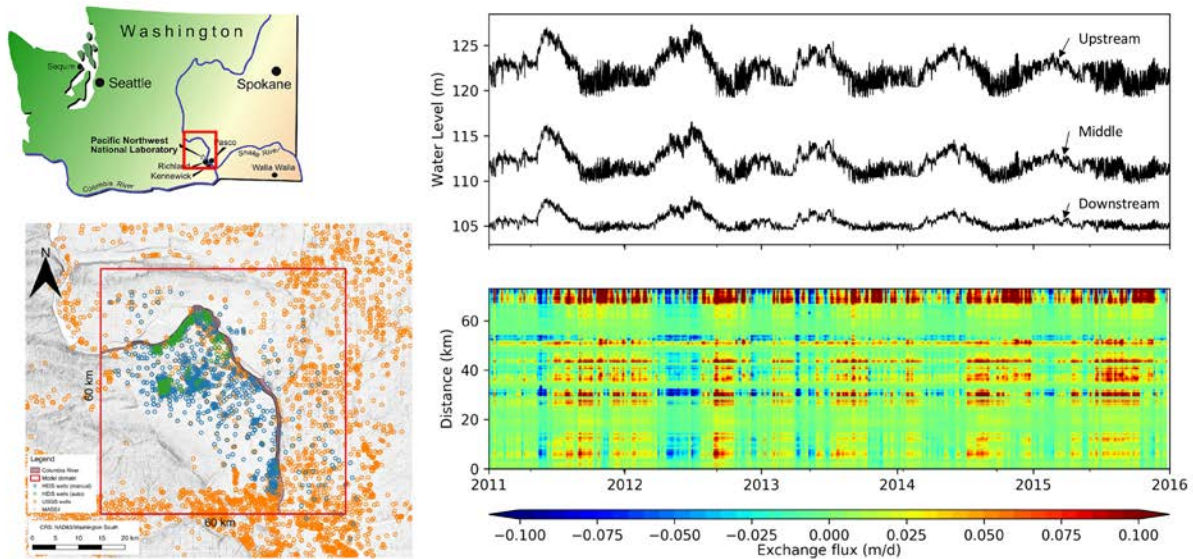


Figure 3. Model predictions of exchange flux over the 70-km Hanford Reach under variable river flow conditions. Upper left: Map showing location of the Hanford Reach within Washington State. Lower left: detail map of the Hanford reach showing groundwater well control data used to set up the PFLOTRAN simulations. Upper right: River stage at three locations across the Reach over the time period simulated (2011-2016). Lower right: Plot of exchange flux (HEFs) over time (horizontal axis) and space (vertical axis, where 0 = tailrace of Priest Rapids Dam and 70 = lower (downstream) end of the Hanford Reach). This plot clearly indicates the variability of estimated HEFs at multiple spatial and temporal scales.

At the km-scale, the exchange pathways exhibited strong heterogeneity along the river shoreline as impacted by the physical heterogeneity in riverbed substrate and in the aquifer. The riverbed permeability (or conductance) and its spatial heterogeneity were identified as the most sensitive parameters of the HEF model. The exchange patterns also varied substantially with changes in river stage at multiple temporal scales (Figure 3). Consequently, the residence time distribution of river water in the groundwater system featured long tails and multiple modes. Strong inter-annual variability in river gaining/losing conditions was revealed in multi-year simulations. High-frequency flow variations were found to enhance spatio-temporal variability of HEFs and increase total exchange volumes.

Initial river corridor module development and testing revealed significant control of HEFs on stream nitrate fluxes: Development of our river corridor module started with coupling three components: (1) SWATR enhanced with a multi-rate mass transfer (MRMT) mechanism, (2) Networks with EXchange and Subsurface Storage (NEXSS; (Gomez-Velez and Harvey, 2014)) model for steady state HEFs and residence time distribution, and (3) PFLOTRAN biogeochemistry for simulating reactive transport within the river corridor. The NEXSS model yields much larger vertical exchange fluxes than lateral exchange fluxes based on steady state assumptions, which motivates planned modifications that consider dynamic flow conditions. Application to the Upper Columbia-Priest Rapids watershed yielded residence time estimates along the main stem that ranged from hours to days, whereas cumulative residence times in tributary channels were much larger. However, the magnitude of exchange flux was much greater in the main stem than in tributaries, which offset the effect of residence time such that overall nitrate removal was predicted to be larger in the main stem than in tributary channels. This effect is in contrast to conventional wisdom which suggests that small channels contribute most to nutrient cycling. Additional model testing and experimental validation is needed to confirm this finding.

SWAT watershed model configured to depict impacts of anthropogenic perturbations on watershed nitrogen cycling: The SWAT model was applied to the Upper-Columbia Priest Rapids watershed to understand how irrigation of the agricultural fields impacts the nutrient inputs to the river network. We have collected a suite of geospatial datasets to characterize the watershed. Topography information was derived from the U.S. Geological Survey (USGS) National Elevation Dataset (NED) (<https://lta.cr.usgs.gov/NED>) with a spatial resolution of 30 meters. Land cover was defined using the U.S. Department of Agriculture (USDA) Crop Data Layer (CDL)¹ with a spatial resolution of 30 meters. We compiled daily climatic data for the period of 1980-2012 from North America Land Data Assimilation System (NLDAS)². In addition, we obtained data describing nitrogen and phosphorus fertilizer application rates³, tillage intensity⁴, and crop management.⁵ Surface water nitrate data from +USGS monitoring stations were used for model evaluation. Numerical experiments to quantify the influence of irrigation practices on evapotranspiration and streamflow in the Upper Columbia-Priest Rapids watershed is underway. We have collected crop specific irrigation water guides and are currently setting the Maximum Allowable Depletion (MAD) to match simulated and reported irrigation water demand for corn, potato, wheat, and hay.

Quantifying response of ecosystem-atmosphere interactions to HEFs and climate variability along the Columbia River corridor: Our external collaborator, Dr. Heping Liu (Washington State University) and his team worked with the PNNL SFA field crew to install a third flux tower on 13-15 Nov 2017 at the Hanford 100H Area to facilitate cross-site comparisons. The WSU team has investigated how access to groundwater by plants (controlled by water table depth) influences water availability and thus the seasonal patterns of net ecosystem exchange of CO₂ (NEE) and evapotranspiration (ET) at two semi-arid ecosystems along the Columbia River corridor. We examined one year of eddy covariance measurements from an upland sagebrush ecosystem without groundwater access (deep water table, 300 Area) and a

¹ <https://nassgeodata.gmu.edu/CropScape/>

² <https://ldas.gsfc.nasa.gov/nldas/NLDAS2forcing.php>

³ <https://www.ers.usda.gov/data-products/fertilizer-use-and-price.aspx>

⁴ <http://www.ctic.org/resourcedisplay/255/>

⁵ <http://usda.mannlib.cornell.edu/MannUsda/viewDocumentInfo.do?documentID=1251>

riparian grassland ecosystem with access to groundwater (shallow groundwater influenced by river intrusion, 100H Area). The two sites exhibited distinct seasonal patterns of NEE and ET, driven by differences in water availability between the two sites. While NEE at the upland sagebrush site was strongly constrained by water availability during the dry summer months, access to groundwater allowed the riparian site to maintain high NEE magnitude and ET during the same dry period. In 2016, the riparian site had larger annual gross primary productivity (GPP) than the upland site (612 versus 424 gC m⁻²), which was offset by higher ecosystem respiration (558 versus 363 gC m⁻²). Thus, the magnitude of the annual NEE at the upland site was larger than that at the riparian site (-62 versus -54 gC m⁻²). Our results demonstrated that groundwater access to plants, controlled by water table dynamics related to connectivity between groundwater and surface water, could be a critical driver of carbon uptake and evapotranspiration in semi-arid ecosystems.

Plans for FY19

We will continue to refine our reach-scale, river corridor and watershed-scale models in FY19, integrating field observations at those scales to enable the model-data integration cycle. A reach-scale thermal model will be built based on the reach-scale hydrologic model. We will work with Campaign B on developing highly mechanistic OPENFOAM-PFLOTRAN simulations at multiple hydromorphic units and work with Campaign C to link thermodynamic characteristics of organic carbon with field-scale biogeochemical modeling driven by HEFs. CLM-PFLOTRAN will be set up at the reach scale to investigate the impacts of HEFs on land-surface fluxes.

Research Campaign B (RC-B): Mechanistic Models

Overall Objectives: *The Mechanistic Models Campaign aims to reveal hydrobiogeochemical processes governing distributions of HEFs, residence times, and reaction rates, and contribute to establishing their appropriate representation in larger-scale models.*

- Characterize and classify hydromorphic and hydrogeologic structures in a manner that is general, measurable using commonly available data, and transferable to other river systems.
- Quantify the influence of hydromorphic structure, hydrogeologic heterogeneity, and variable river discharge on HEFs, surface water residence times, and biogeochemical reaction rates.
- Quantify first-order characteristics of system behavior at the hydromorphic structure scale in support of reduced-order model formulation and parameterization at the reach scale.

Key Contributions of this Research Campaign to the SFA: The resulting process knowledge will contribute to the resolution of Science Question 1 in collaboration with RC-C. The resulting model outputs will contribute to the resolution of Science Question 2 in collaboration with RC-A. To do so, RC-B will develop high-resolution mechanistic models of HEFs and associated reactive transport processes. Simulations of HEFs, residence time distributions, and reactive transport will be performed for a variety of hydromorphic/ hydrogeologic conditions and under variable river discharge conditions. Campaign activities are built around the central theme of using mechanistic model outputs of system components (hydromorphic structures) to identify characteristic component behaviors and parameterize reduced-order models at reach and watershed scales. Model results will inform RC-A development and parameterization of reach-scale reduced-order models of transport and biogeochemical transformation of key carbon and nitrogen species. Where relevant to contaminant plumes, model results will also support RC-A interpretation of observations of contaminant transport and implications for large-scale hydrologic exchange. Mechanistic models will be underpinned by and tested against observational and experimental data from RC-C. Hydromorphic classification maps will guide RC-C experimental design and field site selection.

FY18 Research Targets

FY18 Science Plan Milestone: Develop reach-scale hydromorphic classification scheme and map hydromorphic features across the Hanford Reach. Identify canonical hydromorphic features for detailed study in collaboration with RC-C. Identify suite of river discharge scenarios in collaboration with RC-A. Develop high-resolution modeling workflow and apply to canonical features with homogeneous hydrogeology. Initiate development of new reaction modules incorporating historical contingencies and DOC character (via feedbacks with RC-C). Initiate high resolution reactive transport simulations.

Progress Brief for FY18

Activities have focused on development and application of a reach-scale hydromorphic classification scheme. The classification results were successful and have been used in collaboration with RC-A and RC-C to define specific sub-reaches and hydromorphic features to which high-resolution mechanistic modeling is being applied. We have developed and tested a modeling workflow for integrating surface and subsurface 3D high-resolution flow models and are now applying that workflow to evaluate the impacts of hydromorphology and variable river discharge on HEFs and subsurface residence time distributions. We have developed new microbial reaction networks that incorporate the effects of inundation history and mixing of pools of variable organic carbon character. Key elements of progress and associated scientific findings are as follows:

Reach-scale hydromorphology can be accurately classified by combining bathymetric and hydrodynamic simulation data: We significantly extended the hydromorphic classification approach of Wyrick et al. (2014) to develop a broadly applicable, objective methodology that is based on integration of geospatial data with hydrodynamic simulations. Wyrick et al. (2014) used 2D hydrodynamic simulations of steady river flow to create water depth and velocity maps of a target reach. They then prescribed a mapping of velocity-depth combinations to hydromorphic feature types based on expert knowledge. We eliminated the subjectivity of this approach by applying an unsupervised machine learning method to define the mapping, and included additional variables, to “let the data speak for themselves.” Our approach also considers variability of river flow over a long time period rather than assuming a single steady flow condition. We found that the new approach accurately defines seven distinct hydromorphic feature types and enables automated mapping of those features at the reach scale

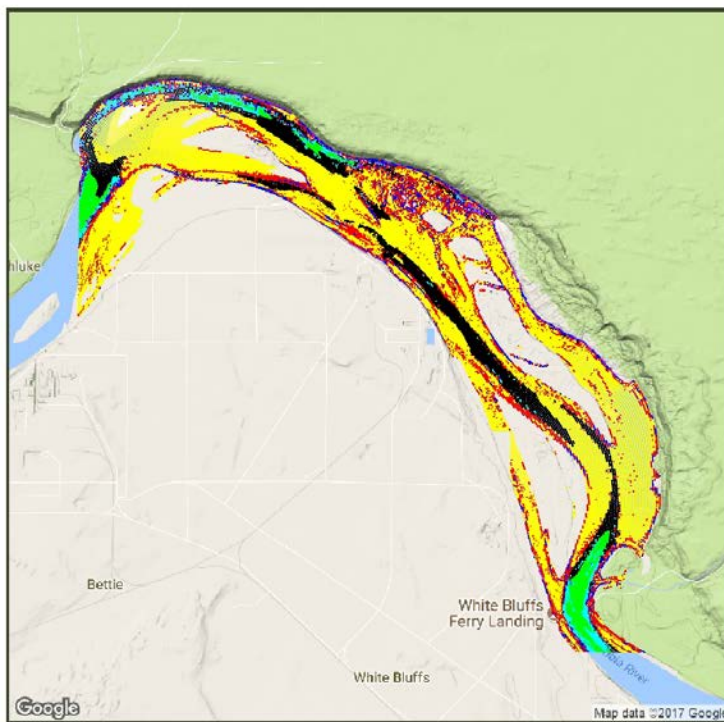


Figure 4. Map of seven hydromorphic unit classes in a 7-km stretch of the Hanford Reach near the 100H and 100F Areas. Black=Fast Glide (21%); Red=Slow Glide (16%); Green=Pool (11%); Blue=Deadwater (<1%); Cyan=Transition (1%); Purple=Slack Water (7%); Yellow=Riffle (44%). We have mapped the entire Hanford Reach but only a segment is shown here for visual clarity.

(Figure 4). Together with emergent bar (island) surfaces, these features completely map the river channel, and correspond well with accepted characteristics of conventionally-defined hydromorphic features [e.g., (Wheaton et al., 2015)]. These maps have been used to select several sub-reaches for high-resolution coupled surface-subsurface flow modeling. The selection process also considered preliminary outputs from reach-scale modeling of RC-A and field site selection and permitting from RC-C. A manuscript describing the classification method and results is currently in preparation.

Coupled Surface-Subsurface High-Resolution Flow Modeling: We developed and tested a coupled surface flow / subsurface flow modeling workflow. The 3D river hydrodynamics is simulated using the open source OpenFOAM code, applied at high resolution (20 m horizontally, 1 m vertically) using LIDAR bathymetry as input. Boundary conditions are provided from the 1D simulation outputs from the PNNL code MASS1, previously calibrated for the Hanford Reach over the historical flow period. OpenFOAM outputs time series of dynamic pressures over the riverbed surface, which are subsequently used as boundary conditions to drive PFLOTRAN simulations of subsurface flow in the river corridor. The coupled OpenFOAM/PFLOTRAN modeling workflow was tested and validated using a sequence of test problems ranging from a simple planar surface synthetic model to the 400-m domain Hanford 300A simulations performed by RC-A (Song et al. in review) to a 7-km sub-reach (Zhou et al., 2018). We found that the coupled model workflow was able to efficiently perform 3D high-resolution simulations of coupled flow over sub-reaches several kilometers in length and over time periods of one year or more using available HPC resources. This workflow is currently being applied to several sub-domains within the Hanford Reach, corresponding to a variety of hydromorphic settings selected based on the classification results described above and to areas being targeted for field research in RC-C. Three flow scenarios are being simulated, corresponding to high, medium, and low-flow years. The PFLOTRAN flow solution will be used as input to a particle tracking model previously developed under this project, which will be applied to compute subsurface residence time distributions.

New reaction networks represent biogeochemical impacts of hydrologic history and carbon character: Based on studies conducted by RC-C, we are developing new reaction network models that incorporate effects of historical contingencies and carbon character. These new reaction networks will be integrated into PFLOTRAN for use in reactive transport simulations at hydromorphic feature scale (this Campaign) and reach scale (RC-A). A model was developed that represents the effects of inundation history on microbial respiration. This model conceptualized two groups of organisms, copiotrophs that predominate under high carbon inputs (inundated conditions) and oligotrophs that predominate under low carbon inputs (dry conditions). By simulating the dynamics of these two groups, we found that it is possible to simulate a time lag in response to re-inundation that depends on the prior inundation history, as observed in RC-C experiments (Goldman et al., 2017). The second element of reaction network development focused on modeling the effects of mixing two pools of organic carbon (groundwater and surface water). This model builds on previous enzyme-based networks (Song et al., 2017) by accounting for the optimal generation of enzymes to degrade labile and recalcitrant carbon pools. The model was able to reproduce the effects observed in RC-C experiments (Stegen et al., 2018) in which carbon respiration occurred only within a certain range of mixtures of surface water and groundwater. A third element of reaction network development is leveraging the capabilities of KBase⁶ to construct metabolic networks based on genomic and metabolomics data. This novel approach provides reaction networks that can represent the metabolic capacity of hyporheic zone microbial communities at varying levels of complexity.

Plans for FY19

In FY19 we will continue to apply our coupled mechanistic modeling workflow to targeted sub-reaches. As field observations become available from RC-C, we will use those data to test, validate, and refine parameterizations for our simulations. Simulation complexity will be systematically increased, first incorporating heterogeneity at the formation scale (alluvium, Hanford-Ringold contact) and then

⁶ <http://kbase.us>

incorporating sub-formation-scale heterogeneity. Outputs from flow and transport modeling will be analyzed to assess the role of hydromorphic features in controlling residence time distributions and to identify other controlling factors. We will continue to develop and advance new reaction network models as experimental observations are obtained by RC-C, and will incorporate those new networks into PFLOTRAN simulation at the hydromorphic unit scale. We will work with RC-A to formulate and parameterize reduced-order (multirate mass transfer) models to be applied at reach and watershed scales.

Research Campaign C (RC-C): Process Studies

Overall Objectives: The Process Studies Campaign is focused on understanding the processes underlying interactions among biogeochemical function, variable discharge, hydromorphology, and hydrogeology.

- Reveal how the history of inundation dynamics (e.g., inundation return frequency) influences the timescales of microbial and biogeochemical responses to re-inundation in a dynamic river stage systems, with a focus on aerobic metabolism in the parafluvial zone.
- Reveal processes governing the character (e.g., thermodynamic favorability and/or bioavailability) of DOC along subsurface flow paths and the influences of DOC character on microbial communities and rates of aerobic metabolism.
- Translate concepts and knowledge - related to inundation history and DOC character - into biogeochemical reaction networks through interactions with RC-B3.1.
- Provide robust spatiotemporal data streams for representative locations along the reach that will 1) facilitate model calibration/evaluation from local to reach scales; and 2) link HEFs and rates of aerobic metabolism to hydromorphic and hydrogeologic settings, through iteration with RC-B.

Key Contributions of this Research Campaign to the SFA: The resulting process knowledge will—in collaboration with RC-B—contribute to the resolution of Science Question 1. RC-C is primarily performing field and laboratory data collection and experimentation. New conceptual understanding and data products generated by RC-C inform local models in RC-B (e.g., by providing local hydrogeology and measurements of biogeochemical fluxes) and reach-scale models in RC-A (e.g., reach-scale spatiotemporal variation in organic C stocks). Model outputs from both Campaigns A and B inform the design of experiments and monitoring networks (e.g., provide potential mechanisms governing observed reactive solute dynamics). RC-C focuses on aerobic metabolism—including respiration and nitrification—and the influences of DOC character. These processes and features were selected because 1) they have relevance to ecosystem health through influences on endangered anadromous fish, migratory birds, and broader river corridor food webs, 2) DOC delivers energy to drive major subsurface biogeochemical cycles, and 3) groundwater and surface water in our field system are usually aerobic. We have, however, observed anaerobic processes (e.g., denitrification, methanogenesis) in the field system, and will be expanding to new field sites within the Hanford Reach that may be dominated by different sets of processes. Field measurements will therefore include reactive solutes reflective of both aerobic and anaerobic processes (e.g., dissolved oxygen, nitrate, methane), while our manipulative experiments will initially focus on aerobic metabolism.

FY18 Research Targets

FY18 Science Plan Milestone: Operationalize an automated hydrobiogeochemical sampling system and perform hydrogeologic characterization at canonical hydromorphic settings using hydrogeophysical inversion. Initiate reach-scale HEF monitoring and experiments to reveal processes governing DOC character.

Progress Brief for FY18

Significant efforts in FY18 have focused on operationalizing an automated hydrobiogeochemical sampling system, addressing practical and sensor needs for reach-scale HEF monitoring, and conducting manipulative experiments and field-based observational studies focused on the causes and consequences of variation in DOC character. In addition, significant effort has been focused on developing a new distributed research network, referred to by the acronym WHONDERS. Please see the external collaborations section for a summary of WHONDERS. Key elements of progress and associated scientific findings are as follows:

Automated sampling system. The design and installation of an automated system within the Hanford 300 Area has been completed and the system is currently operational. The system autonomously draws water from 62 hyporheic zone and 1 river water sampling tubes - automatically switching among tubes—and sends the sampled water through a series of water chemical and physical property sensors. The sampling tubes are distributed in 3-dimensional space over an approximately 60x10 m plot, with sampling depths at approximately 0.5, 1.0, and 2.0 meters, providing sufficient coverage to enable process understanding and modeling at the mechanistic (hydromorphic unit) scale. The data are automatically logged, thereby providing spatiotemporal characterization of subsurface aqueous biogeochemical conditions. Logged parameters include dissolved oxygen, specific conductivity, nitrate, turbidity, pH, temperature, DOC-equivalent, TOC-equivalent, oxidation-reduction potential, and hydrogen sulfide. The ability to collect physical samples from the system was recently added, whereby subsets of sampling tubes are selected for the collection of water samples to evaluate science questions associated with spatiotemporal variation in DOC character. These physical samples are also analyzed for water quality parameters, thereby serving to ground-truth sensor performance. Collection and analysis of the physical water samples is ongoing. In addition to spatiotemporal monitoring of water quality and enabling collection of physical water samples, the automated system contains thermistors associated with each sampling tube. Data from the thermistors are logged at 5 minute intervals, which provides high resolution temporal dynamics of the 3-dimensional thermal field throughout the sampled domain. The thermistors also serve as geophysical electrodes capable of doing static as well as time-lapse electrical resistivity tomography (ERT). To date, the electrode array has been surveyed nearly 1000 times both under baseline and transient conditions. Geophysical inversion of the resulting data have provided both static and dynamic 3-dimensional images showing significant spatial heterogeneity in sediment conductance and hydrologic exchange. These data provide detailed subsurface hydrogeologic characterization that is essential for rigorously constraining highly-resolved reactive transport models at the hydromorphic unit scale (RC-B). This is a core foundation for linking from the hydromorphic unit scale (RC-B) to reduced order models at reach-to-watershed scales (RC-A).

Multi-sensor probe for reach-scale HEF monitoring. Activities under RC-B are characterizing hydromorphic features along the Hanford Reach that RC-C will instrument for estimating HEFs. Current groundwater/surface water flux monitoring approaches estimate either transient pore fluid velocity or mass flux rate at the surface water/groundwater interface, but not both. To address this limitation, we are developing a multi-sensor probe (Figure 5, left image) that continuously monitors the vertical distribution of pore fluid conductivity, temperature, pressure, and bulk electrical conductivity. Combined with fluid conductivity, bulk electrical conductivity estimates the vertical distribution of porosity, which links pore fluid velocity to mass flux. We developed the capability to simulate all time-series data from the probe using PFLOTRAN-E4D, and a joint Occam's inversion for estimating the simplest vertical distribution of porosity, permeability, and dispersivity that honor the data. We also developed a companion stochastic analysis to investigate uncertainty in parameter estimates and corresponding flux rates. Once parameters are estimated, transient pore fluid velocity and mass flux can be monitored using only the pressure sensors located at the top and bottom of the sensor probe. The sensor probe is currently being tested in the laboratory in a 1.5m-tall column (Figure 5, right image). Results from all four data types are very promising. These data will be modeled and compared against known conditions imposed within the test column to validate the multi-sensor probe performance.

Causes and consequences of variation in DOC character. Multiple field-based studies from the SFA have shown important influences of DOC character on hyporheic zone biogeochemical function (Graham et al., 2018; Graham et al., 2017; Stegen et al., 2018). To evaluate specific hypotheses derived from these field studies we developed a non-invasive method to measure sediment oxygen consumption using fiberoptic sensors. This allows us to analyze differences in metabolic rates within hyporheic zone sediments in response to changes in DOC character and concentration using batch incubations. We studied four compounds characteristic of groundwater (i.e. serine, ascorbate) and surface water (i.e. lysine, propionate) at three different concentrations (1X, 10X, 30X). Analysis revealed no significant relationship between respiration rates and the character of added DOC, though concentration effects were significant. This indicates that microbial communities were able to rapidly alter their metabolic machinery to oxidize the different DOC substrates. Multi-omic analyses are being pursued to reveal how microbial communities regulate/shift the expression of metabolic pathways to maintain consistent overall respiration rates despite changes in DOC characteristics. Results will inform further development of regulation-based biogeochemical reaction networks for inclusion in PFLOTRAN simulations at the hydromorphic unit scale (RC-B), and in turn, the representation of DOC character in larger scale reduced order models (RC-A).

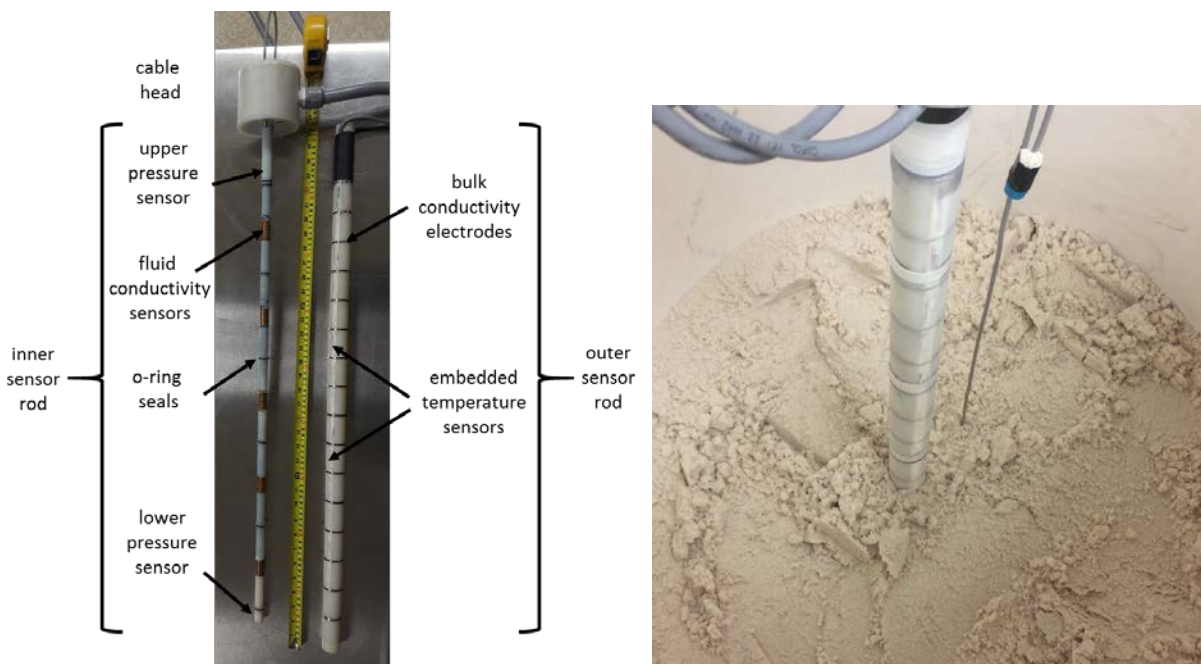


Figure 5. Left: Sensor rod with components labeled. Right: Installation of sensor rod in large column for validation testing.

Plans for FY19

In FY19 we will continue to examine influences of DOC character, but significant effort will be placed on conducting manipulative experiments and field studies examining the influences of hydrologic history on system responses to future hydrologic perturbations. We will continue to operate and sample from the automated sampling system while significantly expanding our use of conservative and reactive tracer studies that use that system. We will deploy the multi-parameter sensor system to hydromorphic features around the Hanford Reach as well as freely providing this technology to WHONDRS collaborators. Another focal area will be significant expansion of WHONDRS to hyporheic zone sampling, distributed incubations, and inclusion of additional sensors.

Select Science Highlights from Research Campaigns

Research Campaign A - Simulating Interactions among River Water, Groundwater and Land Surfaces by Coupling Different Models: Many Land System Models (LSMs) do not consider lateral transport of water, leaving out a cross-sectional view and understanding of the coupling of surface water with groundwater along rivers, streams, and other water bodies. However, detailed observational studies and their accompanying model simulations suggest that the lateral flow of water in the subsurface along the continuum between river water and groundwater saturates the pore space in the soils and sediments. There is a need to advance large-scale LSMs so that they capture the variable gradient of water within soils because this is critical for understanding and modeling energy and water budgets, as well as biogeochemical cycling in the terrestrial surface and subsurface systems. This work enables this modeling advance by coupling a widely used, massively parallel multiphysics reactive transport code (PFLOTRAN) with the Community Land Model (CLM) version 4.5 to create a coupled model called CP v1.0. This open-source coupled model can be used to improve the mechanistic understanding of ecosystem functioning and biogeochemical cycling along river corridors and their functions in watersheds. The associated dataset from a well-characterized river shoreline site can also be used as a benchmark for testing other integrated models.

Reference: Bisht, G., M. Huang, T. Zhou, X. Chen, H. Dai, G. E. Hammond, W. J. Riley, J. L. Downs, Y. Liu, and J. M. Zachara: Coupling a three-dimensional subsurface flow and transport model with a land surface model to simulate stream–aquifer–land interactions (CP v1.0), *Geosci. Model Dev.*, 10, 4539–4562, doi:10.5194/gmd-10-4539-2017, 2017.

Research Campaign B – An enzyme-based approach to simulating microbial metabolism: Key processes that drive biogeochemical dynamics and functions are poorly understood and underrepresented in ecosystem models. Experimental data and field observations often show complex biogeochemical dynamics (e.g., a long time delay in enzymatic response to environmental changes) that have not yet been embodied in numerical models of microbially-mediated reactions. Motivated by an observation of such time lags in denitrification experiments, we developed a new concept of microbial community modeling that explores an underlying mechanism and the interactive dynamics between enzymes and nutrients. Whereas typical approaches account for individual dynamics of species or their groups (called functional guilds), the new model provides a collective description of community function based on functional enzymes as informed by metagenomics information. This new concept is scalable to structurally complex microbial communities because there is no need to parameterize the dynamics of species guilds. Additionally, the model accounts for microbial regulation, which is important, but has been paid little attention until now. We demonstrated that the resulting model can simulate a time lag of several days in enzymatic responses as was observed in experimental studies. Further, the model reveals that the delayed enzymatic reactions could be primarily controlled by transcriptional responses and that the dynamics of transcripts and enzymes are closely related. This model provides a foundation for additional reaction network modeling currently underway, that will in turn inform mechanistic simulations of reactive transport at hydromorphic unit and reach scales.

Reference: Song, H-S., D. Thomas, J. Stegen, M. Li, C. Liu, X. Song, X. Chen, J. Fredrickson, J. Zachara and T.D. Scheibe, Regulation-structured dynamic metabolic model provides a potential mechanism for delayed enzyme response in denitrification process, *Frontiers in Microbiology*, 8, 1866, doi:10.3389/fmicb.2017.01866, 2017.

Research Campaign C - Influences of organic carbon speciation on hyporheic corridor biogeochemistry and microbial ecology: A Nature Communications paper on the coupled river–subsurface ecosystem describes new insights into the dynamics of mixing groundwater (GW) and river water (RW) and its biogeochemical and microbial effects. It proposes a novel four-part thermodynamic mechanism underlying stimulated biogeochemical activity in the hyporheic zone, in response to GW–RW mixing. To date, there is no full accounting of the mechanisms that prompt and control the

biogeochemical impacts of GW-RW mixing. This weakens the present utility of process-based models built to predict the impacts of environmental change on river corridor ecosystems. This paper helps resolve this shortcoming by improving our understanding of the mechanisms governing DOC transformations and provides a new way to conceptualize the role of thermodynamics. Its findings also provide a way to customize modeling frameworks for these types of systems, leading to improved predictions of how ecosystems respond to environmental change. A key challenge is linking fine-scale processes with larger-scale phenomena. One mechanism commonly thought to enhance the biogeochemical impacts of GW-RW mixing activity is how electron donors join with electron acceptors. This joining results in biogeochemical “hotspots.” Our study proposes an alternative 4-part mechanism governing impacts of GW-RW mixing: (1) Individual molecules of DOC in GW are more thermodynamically favorable for microbial transformation, (2) Low DOC concentrations in GW protect these thermodynamically favorable DOC molecules, (3) DOC in RW is at higher concentrations, but each DOC molecule is less thermodynamically favorable for microbial transformation. This lower favorability protects DOC molecules in RW, and (4) GW-RW mixing stimulates the transformation of DOC to CO₂ by combining GW’s low-concentration, but more favorable DOC, with RW DOC that is higher-concentration but less favorable for microbial transformation. Such thermodynamic mechanisms may strongly influence biogeochemical and microbial dynamics across river corridor ecosystems. The new study furthermore paired the DOC analyses with microbial data and time-lapse electrical resistivity tomography to examine system-scale influences of the finer-scale molecular and biogeochemical processes. This revealed links between ecological drivers of microbiome composition, DOC biochemistry, and system-scale hydrology and DOC dynamics. Presently, the research team is building these connections into process-based models to predict the impacts of environmental change on river corridor hydro-biogeochemistry (addressing Science Question #1).

Reference: Stegen, J. C., T. Johnson, J. Fredrickson, M. J. Wilkins, A. Konopka, W. C. Nelson, E. Arntzen, W. B. Chrisler, R. K. Chu, S. Fansler, E. Graham, D. Kennedy, C. T. Resch, M. Tfaily, and J. M. Zachara, Influences of organic carbon speciation on hyporheic corridor biogeochemistry and microbial ecology, *Nature Communications* 9(1): 585, doi:10.1038/s41467-018-02922-9, 2018.

Publication Analysis

45 peer-reviewed journal articles and one peer-reviewed book chapter have been published or are in press in 2017 and 2018 to date (see Appendix A for a complete list). Over this period, the SFA published most frequently in two journals, each with six papers: *Water Resources Research* and *Environmental Science & Technology*. These two journals are among the top-ranked in their respective fields, with WRR being #1 in Limnology and #4 in Water Resources, and ES&T #4 in Environmental Engineering. Outside of these two journals, the remaining 33 papers were published in 30 different journals, reflecting the diversity of SFA research and the wide audience reached by our publications. The SFA publishes in high-quality journals: One 2018 publication is in a DOE-designated high-impact journal, *Nature Communications*, and 83% of the publications are in ISI-designated top quartile journals in their respective fields. The average impact factor of the journals for which data are available (weighted by the number of SFA papers published in each) is 4.39.

Future Scientific Goals, Vision, and Plans for Meeting Program Objectives

*The overarching objective of Subsurface Biogeochemical Research is to advance a robust, predictive understanding of watershed function and response to perturbations as needed to address U.S. energy and environmental challenges.*⁷

The long-term vision of the SFA, closely aligned with the SBR program objective stated above, will culminate in the creation of a new broadly applicable community Earth system simulation capability to predict critical hydrologic, biogeochemical, and ecological processes in the river corridor, linked with

⁷ https://doesbr.org/documents/SBR_Brochure.pdf

other watershed hydrobiogeochemical system component models to provide predictive understanding of watershed function. In the current Triennial Period (FY18-20) we are expanding our previous field research to multiple field sites around the Hanford Reach and linking a multi-reach river corridor model with a model of the Priest Rapids-Upper Columbia watershed. We are also engaging the international scientific community to develop a new collaborative network that will provide new understanding of how our Hanford Site studies fit into the context of other dynamic river and watershed systems. In the next Triennial Period, we will further expand the scope of our research to incorporate biogeochemical processes in Columbia River impoundments and application of our models to expanded watershed areas, and continue to strengthen broad collaborations to support the generalization of our results to other systems of interest. By the end of the next Triennial Period we aim to have fully developed an integrated watershed – river corridor modeling capability with a strong foundation in mechanistic understanding of river corridor hydrology and biogeochemistry, and initiated efforts to integrate that capability with larger-scale modeling systems such as E3SM and the National Water Model.

New Scientific Results that may Shift Current Research or Motivating Knowledge Gaps

FY18 is the first year of the current Triennial Period for which our research plan was reviewed in 2017. The plan is currently being implemented as written and no significant changes in direction or activity plans have been identified at the current time. We have significantly expanded our collaborative efforts, particularly through the WHONDRS network, to build understanding of how processes observed in our system relate to processes in river systems with differing characteristics. We expect that the large body of observations that will be made through WHONDRS will reveal new system behaviors and identify additional gaps in understanding.

Collaborative Research Activities

Direct-Funded Collaborations – The SFA directly funded the following external collaborations during FY17 and FY18: These collaborations are all continuing with the exception of Roden, whose funding period ends in FY18.

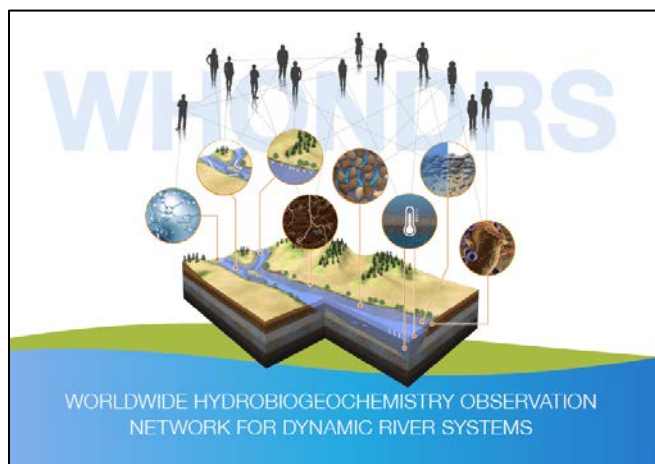
- Heping Liu, Washington State University – Install, maintain, and process data from eddy flux towers at multiple locations along the Hanford Reach for RC-A.
- Gautam Bisht, Lawrence Berkeley National Laboratory – Collaborate with RC-A on linking CLM with PFLOTRAN, and test performance with various interaction zone and climate scenarios.
- Glenn Hammond, Sandia National Laboratory – Support PFLOTRAN development and implementation in RC-A and RC-B, including incorporation of new reaction network models.
- Eric Roden, University of Wisconsin – Investigate carbon sources driving microbial activity in the subsurface interaction zone.
- Jesus Gomez-Velez – Apply the NEXSS model to our experimental system (Hanford Reach and Priest Rapids – Lower Columbia Watershed) and work with RC-A and RC-B to incorporate new mechanistic understanding into NEXSS and couple it with other watershed modules.

SBR-Funded University Collaborations – The SFA collaborates closely with three university-led projects funded by the SBR program. A brief statement of collaborative activities for each is provided here:

- Bayani Cardenas (University of Texas Austin): Performing laboratory flume studies of HEFs and biogeochemistry in dynamic flow systems. We have provided biogeochemical analyses of samples from their flume and regularly coordinate activities to transfer understanding between laboratory and field scales and incorporate new understanding into models. One student from the Cardenas lab is joining the SFA and PNNL through the Pauling Distinguished Postdoctoral researcher program.

- Michael Gooseff (University of Colorado): Performing reach-wide studies of key water quality variables to infer major zones of groundwater efflux into the river at the reach scale. A boat survey and one sampling trip has been completed, and planning is underway for more exhaustive surveys to be conducted in the future.
- Kelly Wrighton (Ohio State University): Investigating processes governing greenhouse gas fluxes in the hyporheic zone of the Columbia River. Field instruments have been installed and one additional sampling trip has been completed. Three additional sampling trips are planned for FY18, with plans to submit a full proposal to the next university-led FOA from SBR.

WHONDRS Network: The Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems (WHONDRS) has been initiated by the SFA as a global consortium of researchers and other interested parties that aims to understand the hydrologic, biogeochemical, and microbial impacts of sustained high-frequency water-level fluctuations in river corridors throughout the world from local to global scales. In the context of the SFA, the purpose of WHONDRS is to place new understanding of river corridor processes developed for our system of focused study (Hanford Reach of the Columbia River)



in the context of other river systems with different properties. While our understanding of dynamic river corridors is increasing, there is still significant uncertainty in the hydrobiogeochemical impacts of sustained high-frequency stage fluctuations, and how those influences vary across systems with different characteristics. This uncertainty (and lack of adequate representation in models) undermines our ability to predict feedbacks among the operation of energy-water systems, water quality, and the health of dynamic river corridors under future environmental conditions at regional, national, and global scales.

WHONDRS' distributed scientific approach is based on providing sampling kits, experimental protocols, and new sensor technology to researchers around the world. In turn, samples are collected, experiments are conducted, and sensors are deployed across systems by a large number of distributed collaborators. Sample analysis and computational modeling of sensor data are performed by WHONDRS (in collaboration with EMSL) such that data products are generated in a highly consistent manner across systems. WHONDRS is working with both EMSL and ESS-DIVE to store all raw and processed data and metadata - which are all generated in a highly consistent manner and undergo rigorous quality assessment - into a publicly accessible data archive. This partnership among WHONDRS, EMSL, and the scientific community is based on small contributions from many researchers and is highly scalable. These numerous small contributions accumulate into a large compendium of data and knowledge, from which general principles can be derived.

The primary scientific focus of WHONDRS examines the impacts of high-frequency stage fluctuations on hyporheic zone hydrobiogeochemistry, but WHONDRS is also interested in impacts to thermal regimes, nutrient export, primary producers, and physical dynamics of river corridor ecosystems. WHONDRS is currently pursuing two primary efforts: 1) identification of surface water metabolites and their dynamics in response to river stage fluctuations, and 2) developing new sensor technology to estimate sediment porosity and the mass flux of water moving through the hyporheic zone. The metabolomics effort is currently deployed to the scientific community and will provide broad understanding of factors governing the character of organic carbon that may be delivered to hyporheic zone sediments via hydrologic exchange. Such knowledge is essential as we develop hydrobiogeochemical models that explicitly represent the influences of organic carbon character on river

corridor biogeochemical and microbial function. Key scientific questions being addressed include: 1) Is a core metabolome shared across all streams? If so, what types of metabolites are shared and what types are not? 2) Are there aspects of historical discharge dynamics that consistently drive metabolite profiles across systems? 2) Can we create a 'metabolite atlas' similar to the approach used for soil metagenomics? To implement the metabolomics study, a streamlined sampling kit has been designed and is being shipped to WHONDRS members throughout the world. The kit allows for simple, one-time surface water sampling. Samples are shipped back to PNNL for geochemical analysis as well as to EMSL for metabolomics analysis via Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FTICR-MS). At present, approximately 45 sampling kits have been distributed and samples are beginning to arrive back at PNNL. The SFA is working closely with EMSL to define data standards for FTICR-MS data, and will adhere to previously established data standards for water quality parameters (e.g., names and units for cations and anions). Complying with these standards will enable seamless integration between geochemistry and molecular data, as well as field-based metadata such as geographic coordinates and stream hydrographs. The FTICR-MS data standards are furthermore structured to allow direct upload of the processed data into a FTICR-MS visualization app that PNNL/EMSL will soon make publically available. This will allow anyone to rapidly explore the data and to parse the full dataset into subsets of interest, without the need for programming skills. Removing barriers and enabling the community in this way is at the core of WHONDRS. The stream metabolomics study will soon expand to include collection and analysis of the associated microbial communities. This is being done in coordination with Kelly Wrighton (Ohio State University) and a streamlined protocol is currently being tested in her laboratory. Samples will be collected at the same time water samples are collected for the metabolomics study.

The new sensor technology is being developed and is in the lab-testing phase such that it is not yet deployed to the community (see summary under the Campaign C progress section above). We envision that when it is ready several sensor probes will be constructed and loaned to selected collaborators for installation across a range of river environments.

Other Collaborations

- ESS Cyberinfrastructure Working Groups: Co-PI Xingyuan Chen represents the SFA on the Executive Committee, and other SFA team members participate in working group activities.
- FY18 TES university proposals: The SFA collaborated on one proposal to the FY18 TES call, led by Cara Santelli of the University of Minnesota, entitled “Quantifying the impact of anaerobic methane oxidation and hyporheic flux on methane emissions in boreal wetlands.”
- USGS – SFA staff visited USGS offices in Tacoma and Kennewick to initiate collaborative discussions. We are exploring possibilities for joint data collection activities in the Hanford Reach and beyond.
- ESS-DIVE – The ESS-DIVE team visited PNNL in early June to discuss opportunities and needs. A significant portion of the discussions focused around the SFA data archive approach and future needs. A tangible path forward was agreed upon based, in part, on developing an interface that will link the SFA data archive (managed using Velo) to ESS-DIVE via their existing API. This will facilitate transfer of the large number of data files already stored in our Velo repository to ESS-DIVE to enable DOI assignment.

APPENDIX A: PROJECT PUBLICATIONS

2018

Published:

- Graham E., Crump A., Kennedy D., Arntzen E., Fansler S., Purvine S. O., Nicora C., Nelson W., Tfaily M. and Stegen J. (2018) Multi 'omics comparison reveals metabolome biochemistry, not microbiome composition or gene expression, corresponds to elevated biogeochemical function in the hyporheic zone. *Science of the Total Environment*, **642**, 742-753; doi: 10.1016/j.scitotenv.2018.05.256.
- Meile C. and Scheibe T. D. (2018) Reactive transport modeling and biogeochemical cycling. In *Reactive Transport Modeling: Applications in Subsurface Energy and Environmental Problems*, Y. Xiao, F. Whitaker, T. Xu, and C. Steefel (Eds.), Chapter 10, Wiley Press, 485-510.
- Stegen J. (2018) At the nexus of history, ecology, and hydrobiogeochemistry: Improved predictions across scales through integration. *mSystems*, **3**, e00167-00117; doi: 10.1128/mSystems.00167-17.
- Stegen J. C., Johnson T., Fredrickson J. K., Wilkins M. J., Konopka A. E., Nelson W. C., Arntzen E. V., Chrisler W. B., Chu R. K., Fansler S. J., Graham E. B., Kennedy D. W., Resch C. T., Tfaily M. and Zachara J. (2018) Influences of organic carbon speciation on hyporheic corridor biogeochemistry and microbial ecology. *Nature Communications*, **9(585)**, 1-11; doi: 10.1038/s41467-018-02922-9.
- Yan A., Liu C., Liu Y. and Xu F. (2018) Effect of ion exchange on the rate of aerobic microbial oxidation of ammonium in hyporheic zone sediments. *Environmental Science and Pollution Research*, **25**, 8880-8887; doi: 10.1007/s11356-018-1217-x.
- Zhou T., Bao J., Huang M., Hou Z., Arntzen E., Song X., Harding S., Titzler S., Murray C., Perkins W., Chen X., Stegen J., Hammond G., Thorne J. and Zachara J. (2018) Riverbed hydrologic exchange dynamics in a large regulated river reach. *Water Resources Research*, **54**, 2715-2730; doi: 10.1002/2017WR020508.

In Press:

- Graham E. B., Gabor R. S., Schooler S., McKnight D. M., Nemergut D. R. and Knelman J. E. (2018) Oligotrophic wetland sediments susceptible to shifts in microbiomes and mercury cycling with dissolved organic matter addition. *PeerJ*, **6:e4575**, In press; doi: 10.7717/peerj.4575.
- Hall E. K., Bernhard E. S., Bier R. L., Bradford M. A., Boot C. M., Cotner J. B., del Giorgio P. A., Evans S. E., Graham E. B., Jones S. E., Lennon J. T., Locey K. J., Nemergut D., Osborne B. B., Rocca J. D., Schimel J. S., Waldrop M. P. and Wallenstein M. W. (2018) Understanding how microbiomes influence the systems they inhabit. *Nature Microbiology*, Accepted; NMICROBIOL-16020162D.
- Korneev S. V., Yang X., Zachara J. M., Scheibe T. D. and Battiato I. (2018) Downscaling-Based Segmentation for Unresolved Images of Highly Heterogeneous Granular Porous Samples. *Water Resources Research*, **54**, Accepted; Article ID: WRCR23198; doi: 10.1002/2018wr022886.
- Stegen J., Bottos E. and Jansson J. (2018) A unified conceptual framework for prediction and control of microbiomes. *Current Opinion in Microbiology*, Accepted; COMICR_2017_2201.
- Xu F., Liu Y. and Liu C. (2018) A generalized-rate model for describing and scaling redox kinetics in sediments containing variable redox-reactive materials. *Environmental Science & Technology*, Accepted; doi: 10.1021/acs.est.7b06354.

Submitted:

- Bao J., Zhou T., Huang M., Hou Z., Perkins W., Harding S., Titzler S., Hammond G., Ren H., Thorne P., Suffield S., Murray C. and Zachara J. (2018) Quantifying hyporheic exchanges in a large scale river reach using coupled 3-D surface and subsurface computational fluid dynamics simulations. *Hydrological Processes*, In review; HYP-17-0083.

- Graham E., Stegen J., Huang M., Chen X. and Scheibe T. D. (2018) Integrating hydrology, biogeochemistry and ecology to understand hydropower impacts. *Global Change Biology*, Submitted but didn't go out for review; will be resubmitted to Ecology or WRR by 2/12/18.
- Grant S. B., Gomez-Velez J. D. and Ghisalberti M. (2018) Modeling the effects of turbulence on hyporheic exchange and local-to-global nutrient processing in streams. *Water Resources Research*, Submitted.
- Harvey J. W., Gomez-Velez J. D., Schmadel N., Scott D., Boyer E., Alexander R., Eng K., Golden H., Kettner A., Konrad C., Moore R., Pizzuto J., Schwarz G., Soulsby C. and Choi J. (2018) How hydrologic connectivity regulates water quality in river corridors. *JAWRA Aquatic System Connectivity Featured Collection*, Submitted.
- Hou Z., Scheibe T. D., Murray C. J., Perkins W., Arntzen E., Ren H., Mackley R. D. and Richmond M. C. (2018) Identification and mapping of riverbed sediment facies in the Columbia River through integration of field observations and numerical simulations. *Hydrological Processes*, Submitted; HYP-18-0179.
- Missik J., Liu H., Gao Z., Huang M., Chen X., Arntzen E., McFarland D. P., Ren H., Titzler S., Thomle J. and Goldman A. (2018) Groundwater uptake enhances growing season evapotranspiration and carbon uptake in a semi-arid riparian ecosystem. *Journal of Geophysical Research: Atmospheres*, Submitted.
- Nelson W. C., Graham E. B., Crump A., Fansler S., Arntzen E., Kennedy D. and Stegen J. (2018) Gene-level functional redundancy varies across N-cycling pathways in hyporheic microbial communities *Nature Ecology & Evolution*, To be resubmitted.
- Sengupta A., Stegen J., Neto A., Wang Y., Neilson J., Chorover J., Troch P. A. and Maier R. M. (2018) Assessing microbial community patterns under incipient soil formation from basalt. *JGR Biogeosciences*, In review; 2017JG004315
- Singh T., Wu L., Gomez-Velez J. D., Hannah D. M. and Krause S. (2018) Dynamic hyporheic zones: exploring the role of peak-flow events on bedform-induced hyporheic exchange. *Water Resources Research*, Submitted.
- Song X., Chen X., Stegen J., Hammond G., Song H., Dai H., Graham E. B. and Zachara J. (2018) Drought conditions maximize the impact of high-frequency flow variations on thermal regimes and biogeochemical function in the hyporheic zone. *Water Resources Research*, In Review; 2018WR022586-T; doi: 10.17605/OSF.IO/JW4PH.
- Song X., Ye M., Dai Z., Hammond G., Zachara J. and Chen X. (2018) Delineating facies spatial distribution by integrating ensemble data assimilation and indicator geostatistics with level set transformation. *Water Resources Research*, Rejected by Geophysical Research Letters and will be submitted soon to WRR by 2/28/18.
- Stern N., Meija J., Ginder-Vogel M. A., Yang Y. and Roden E. (2018) Dual role of humic substances as electron donors and shuttles for dissimilatory iron reduction. *Environmental Science & Technology*, Submitted; es-2017-06574p.
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APPENDIX B: REFERENCES CITED

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