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Pacific Northwest National Laboratory SFA Annual Report

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

June 2019

Laboratory Research Manager: Charlette Geffen

Principal Investigators: Tim Scheibe (PI), Xingyuan Chen (Co-PI), and
James Stegen (Co-PI), Maoyi Huang (Watershed Coordinator)

Key Staff: Jie Bao, Tim Johnson, Hyun-Seob Song, Chris Strickland, Xuesong Zhang

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PNNL SBR Scientific Focus Area Annual Report FY2019

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

2019 Annual Report

June 30, 2019

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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. We focus on the nature of hydrologic exchange flows (HEFs), defined as the dynamic exchange of water and chemical constituents between river channels and adjacent subsurface environments that comprise the river corridor [*Harvey and Gooseff*, 2015], and the roles of HEFs in river corridor and watershed biogeochemical processes.

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) as shown in Figure 1. SFA team members work on multiple campaigns, campaign activities are jointly coordinated by the PI team, and high-impact publications are targeted that integrate 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 conduced by the Process Studies RC.

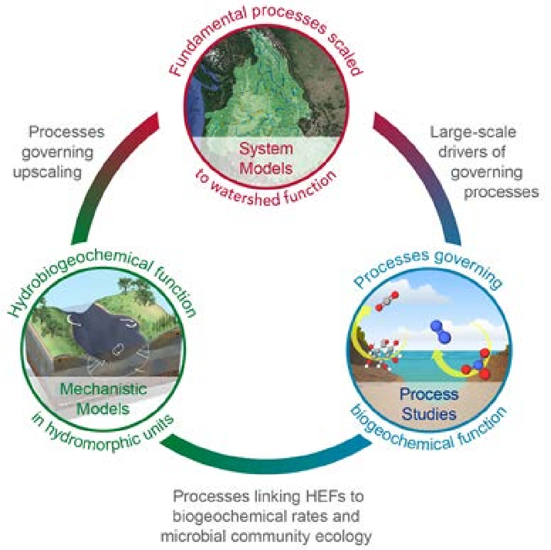

Figure 1 New conceptual understanding from and iterative feedbacks among three Research Campaigns.

- 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 OBJECTIVES

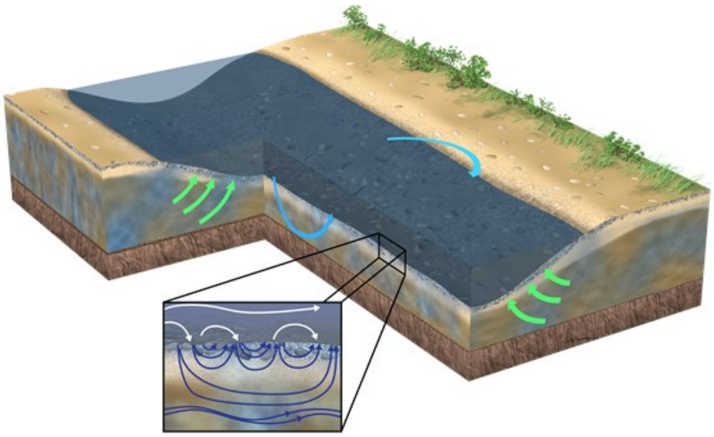

Figure 2. Schematic diagram of different types and scales of Hydrologic Exchange Flows (HEFs), including bedform-driven small-scale vertical exchange (inset) and large-scale bank exchanges driven by temporal variations in river discharge and stage.

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 2) 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 two overarching objectives:

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.

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 objectives 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?
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?

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. 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 3). 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 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 multiple 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.

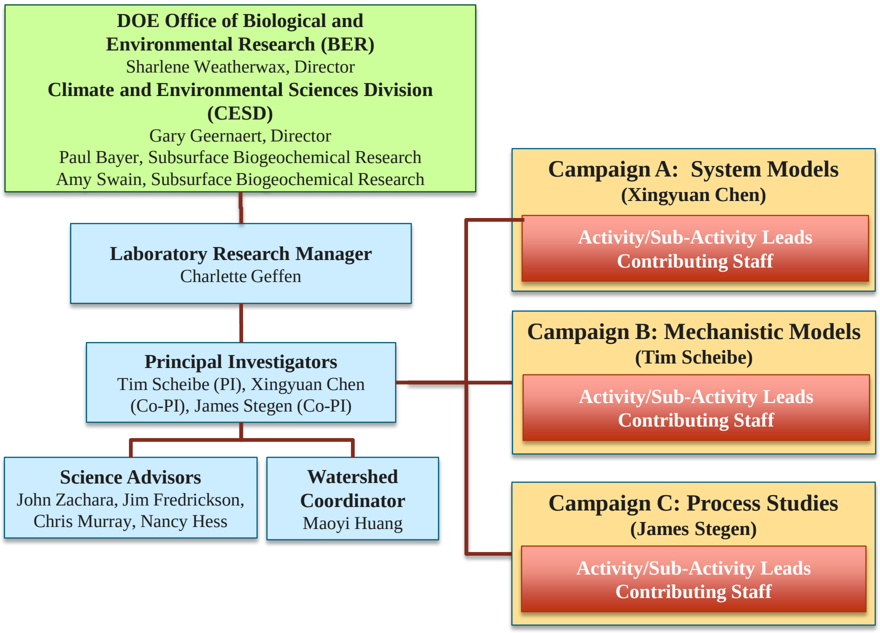

Figure 3. PNNL SBR SFA project team organizational structure.

Our management philosophy and process is characterized by 1) intentional, regular and transparent communication and documentation of progress 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.

FY19 Research Targets

FY19 Science Plan Milestone: Improve the understanding of reach-scale HEFs and associated biogeochemical fluxes by assimilating spatially distributed measurements of HEFs (with RC-C), contaminant tracers, and land surface fluxes into reach-scale models. Incorporate outputs of hydromorphic-scale mechanistic models of HEFs and biogeochemical processes in reduced-order models (with RC-B). Couple PFLOTRAN with SWATR and SWATR with NEXSS. Initial evaluation of watershed biogeochemical fluxes using SWAT.

Progress Brief for FY19

Our activities in FY19 focused on understanding what controls reach-scale HEFs and how HEFs impact contaminant migration, river corridor thermal regimes, land-surface fluxes, and watershed nitrogen cycling, through both numerical modeling and field observations.

(1) *Reach-scale modeling to identify controls on HEFs, thermal regime, and subsurface residence times.* A reach-scale subsurface flow (PFLOTRAN) model, driving in part by time-varying boundary conditions representing variable river stage, revealed that HEFs are largely controlled by channel morphology and subsurface hydrogeology, along with the magnitude and timing of stage fluctuations [*Shuai et al.*, 2019] (see highlight below). This research improves scientific understanding of controls on HEFs at river-reach scale under high-frequency flow variations, an important issue in an era of energetic dam-building worldwide. It also demonstrates the influences of river water intrusion on the migration of groundwater contaminant plumes—particularly for contaminant sources located within the preferential flow paths shaped by ancient river remnants called paleochannels. The PFLOTRAN model was then expanded to incorporate thermal effects, and was used to evaluate the impacts of HEFs on the associated river corridor thermal regime and implications for river ecology. River corridor thermal regime was shown to be strongly influenced by high-frequency flow variations interacting with river temperature dynamics. River corridor thermal regime, like HEFs, exhibited strong spatiotemporal variability. Riverbed temperature lagged behind surface water temperature and the amplitude of riverbed temperature fluctuations was ~60% less than that of surface water. Morphologic features such as islands and gravel bars created areas of upwelling and downwelling that affected the penetration depth of the thermal signal (Figure 4). In general, thermal signals penetrated deeper at the upstream end of morphologic features where strong downwelling occurred. Thermal signals also penetrated deeper where highly permeable sediments existed causing larger exchange flux, creating colder zones in the winter and warmer zones in the summer. Our results demonstrated that upstream dam operations enhanced the exchange between surface water and groundwater and changed river corridor thermal regime with strong potential influence on river ecology. Particle tracking was performed using the velocity field from high-resolution 3D groundwater flow simulations to quantify subsurface residence time distributions (RTDs). The effects of hydrological forcing on RTDs were evaluated by varying river flow boundary conditions

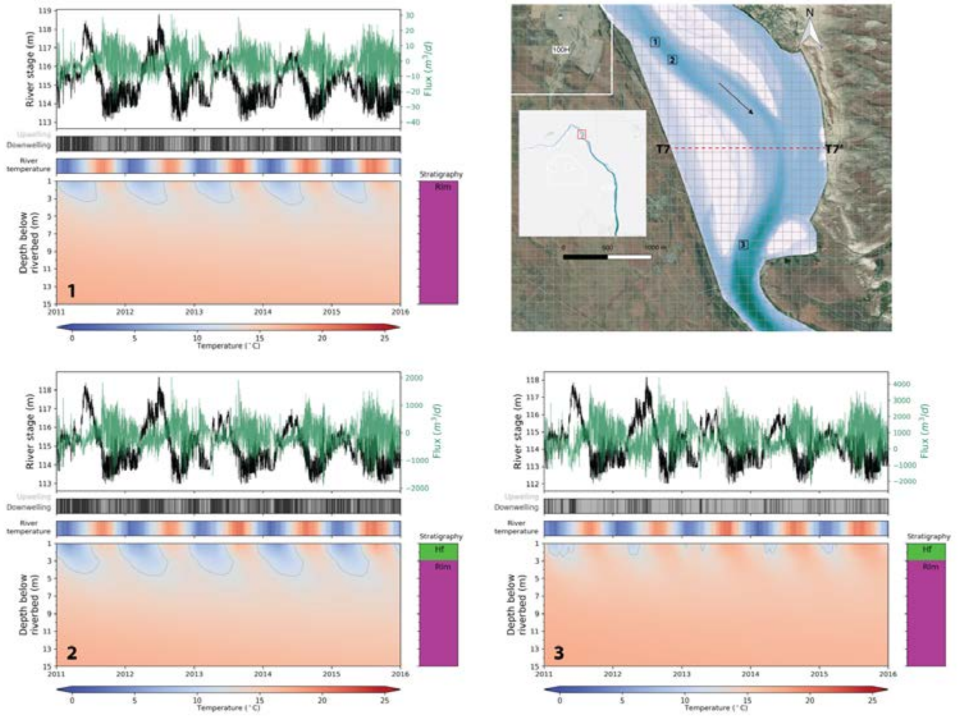

Figure 4 Thermal profiles at three locations around a gravel bar. At each location, river stage, exchange flux and directions, river temperature and vertical stratigraphy are shown. The gray dotted line represents the 12°C temperature contour. Hf--Hanford formation. Rlm--Ringold Lower Mud.

and releasing particles in different time windows. Our results revealed that dynamic stage fluctuations created rapidly changing losing-gaining conditions in the river and led to highly transient, multi-modal RTDs. Dam-induced high-frequency (sub-daily) flow variation contributes to the short-time (sub-daily) component of the RTDs. This analysis showed that multimodal RTDs supported higher biogeochemical reactivity in the hydrological exchange zone relative to unimodal RTDs. Specifically, high-frequency flow variations increased denitrification by 2.6%~18% and aerobic respiration by 14%~18%. Based on these findings, we suggest that current river basin models could be improved by including bank storage and more complex RTD's influenced by both short- and long-term river stage fluctuations. The findings of these reach scale modeling studies are transferrable to other river corridor systems that experience regular, periodic fluctuations.

Publication Highlight: Reach-Scale Model Reveals that Hydrologic Exchange Flow in Large Rivers is Mostly Controlled by Subsurface Hydrogeology: Hydrologic exchange flows (HEFs) increase the contact between river water and subsurface sediments thereby playing a critical role in biogeochemical and ecological functions along river corridors. Yet little is known about the factors that govern the spatial and temporal distribution of HEFs under dynamic flow conditions. A 3-D PFLOTRAN groundwater model of a 60x60 km domain covering the entire Hanford Reach (Figure 5) was used to elucidate the roles of dynamic flow conditions, river morphology, and subsurface hydrogeology in controlling hydrologic exchange flows along this large dam-regulated river corridor. We found that the dominant factors controlling the hydrogeochemical signatures of HEFs along a dam-regulated river reach are river channel morphology and (predominantly) a river channel's subsurface hydrogeology. These features were found to control the locations of high exchange flow rates—"hot spots." Magnitude and timing of river stage fluctuations were found to control the timing of high exchange rates - "hot moments." This research improves scientific understanding of hydrogeomorphic controls on HEFs at river-reach scale under high-frequency flow variations, an important issue in an era of energetic dam-building worldwide. The paper also demonstrates the influences of river water intrusion on the migration of groundwater contaminant plumes—particularly for contaminant sources located within the preferential flow path shaped by ancient, deep river remnants called paleochannels.

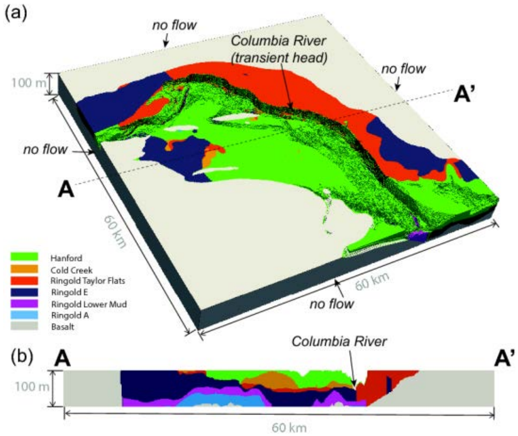

Figure 5 (a) Model domain showing numerous geologic layers. (b) Cross-section showing model complexity.

Reference: Shuai, P., X. Chen, X. Song, G.E. Hammond, J. Zachara, P. Royer, H. Ren, W.A. Perkins, M.C. Richmond, and M. Huang. "Dam Operations and Subsurface Hydrogeology Control Dynamics of Hydrologic Exchange Flows in a Regulated River Reach." 2019. *Water Resources Research*. doi: 10.1029/2018WR024193

(2) *Watershed-scale simulation of biogeochemical dynamics:* Watershed management practices often ignore the potentially important role of hyporheic zones (HZs) as a modulator of water quality. To investigate the effect of hydrological exchange and biogeochemical processes on the fate of nutrients in surface water and HZs, a novel integrated model, SWAT-MRMT-R, was developed within the Soil and Water Assessment Tool watershed model [*Fang et al.*, 2019]. A multirate mass transfer (MRMT) module was integrated with SWAT to model the exchange of water and solute between the river channel and surrounding HZs, modeled as multiple first-order mass transfer processes within different HZ domains. HZs are conceptualized as transient storage zones within the sediments surrounding the river channel where denitrification and aerobic respiration reaction occur. Using an agricultural watershed in Washington State as an example and hyporheic exchange rates and residence times estimated with the basin-scale NEXSS model [*Gomez-Velez and Harvey*, 2014], our simulation results indicate that: 1) only biogeochemically active HZs with residence time on the scale of reaction times can contribute to

significant nitrate removal in surface water; 2) transient storage models that follow a single exchange process rather than a spectrum of exchange processes in each HZ may overestimate the nitrate attenuation role of HZs; and 3) agricultural return flow can cause serious surface water pollution when the exchange between channel and HZs is slow.

We also assessed the hydrological impacts of irrigation practices in agroecosystems using SWAT simulations. Model simulations suggested that irrigation water withdrawal generally reduced streamflow by enhancing water loss through evapotranspiration (ET) in the study area (The Upper Columbia Priest Rapids Watershed) and enhanced nutrient delivery. Results of this study demonstrated importance of incorporating water management activities into hydrologic modeling. Methods and findings from this study will enhance future hydrologic modeling in agroecosystems with intensive irrigation activities.

(3) *Land-surface flux measurements and relationship to groundwater-surface water interactions.* Eddy covariance measurements were used quantify the influence of groundwater-surface water interactions on inter- and intra-annual variability of water, energy, and biogeochemical cycling at three project-funded flux tower sites located on the Hanford site [*Gao et al.*, 2019; *Missik et al.*, 2019]. These flux data were incorporated into the AmeriFlux network that facilitates data sharing and scientific exploration with scientists worldwide; an AmeriFlux site visit was conducted in late June 2019 as the final step of the on-boarding process. We also initiated collaboration with the NASA ECOSTRESS mission (https://ecostress.jpl.nasa.gov/) by sharing observations from the sites and participating in their analyses. The Community Land Model (version 5) was applied at 1-km resolution to quantify effects of irrigation in the Upper Columbia-Priest Rapids (UCPR) watershed. The simulations demonstrated that water and land management practices (e.g., irrigation, fertilization) not only fundamentally change the hydrologic and energy budgets, but also perturb watershed function in carbon and nitrogen cycling in semi-arid regions significantly. The simulation is validated by eddy covariance observations and satellite-based observations in the period of 2000-2018. This work lays the foundation for coupled ELM-PFLOTRAN simulations to quantify the effects of both irrigation and GW-SW interactions on semi-arid watersheds to be conducted in FY20.

(4) *Hydrologic observations and data curation.* A real-time water quality station was established to monitor water quality parameters at an agricultural return flow canal in collaboration with the USGS Mid-Columbia field office. This monitoring station monitors discharge, pH, dissolved oxygen, specific conductance, temperature, and nitrate concentration at 15-min resolution, with all the data made available in real-time on the USGS website https://waterdata.usgs.gov/nwis/uv?site_no=12473503. This continuous dataset will meet a critical data need for watershed model validation. Subsurface data are also critical to model parameterization and validation, and although extensive data have been collected at the Hanford Site, many time series data contain gaps associated with instrument outages and other problems. We explored the ability of deep neural networks to reconstruct data (fill gaps) in spatially distributed time-series data [*Ren et al.*, 2019]. We evaluated the new method using a 10-year spatio-temporal hydrological dataset of temperature, specific conductance, and groundwater table elevation from 42 wells that monitor hydrologic exchanges between the Columbia River and its adjacent groundwater aquifer. We used a long short-term memory (LSTM)-based architecture, which is designed to address both spatial and temporal variations in the property fields. The gap-filling performance was evaluated using test datasets with synthetic data gaps created by assuming the observations were missing for a given time window (i.e., gap length), such that the error could be evaluated from real observations. The performance of the LSTM-based gap-filling method was compared to that of a traditional gap-filling method: autoregressive integrated moving average (ARIMA). Although ARIMA performed slightly better on average error statistics, LSTM was better able to capture nonlinear dynamics present in time series. Thus, LSTMs show promising potential to outperform ARIMA for gap filling in time-series observations characterized by multiple dominant modes of variability, needed to advance understanding of dynamic complex systems.

Plans for FY20

In FY20, RC-A will couple ELM with PFLOTRAN to study the impacts of HEFs on land-surface fluxes; we will couple SWAT-R with PFLOTRAN to establish a river corridor module that incorporates the groundwater component in the river corridor system; we will adopt information theory to evaluate useful information in various reach-scale data for informing reach-scale models and guiding data assimilation to reduce uncertainty in reach-scale hydrologic and thermal process models. We will apply reach-scale particle tracking and incorporate OC characteristic in reach-scale biogeochemical modeling.

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.

FY19 Research Targets

FY19 Science Plan Milestone: Complete simulation of heterogeneous hydrogeologic properties for canonical hydromorphic features and evaluate against geophysical observations from RC-C. Perform high-resolution flow modeling for heterogeneous properties, spatially variable hydrologic head boundaries (with RC-A), and variable river stage, and test against RC-C observations of HEFs. Complete new reaction modules incorporating DOC character (feedback with RC-C) and implement in PFLOTRAN to link variable stage and HEFs to biogeochemical rates.

Progress Brief for FY19

Activities have focused on 1) end-to-end validation of a modeling workflow for integrating surface and subsurface 3D high-resolution flow models; 2) application of that workflow to evaluate the impacts of hydromorphology and variable river discharge on HEFs and subsurface residence time distributions as well as to guide new field instrumentation activities, and 3) development of new microbial reaction networks for aerobic respiration and nitrogen cycling using novel methods for integration of metabolomic and metagenomic information. Key elements of progress and associated scientific findings are as follows:

(1) Coupled Surface-Subsurface High-Resolution Flow and Transport Modeling: We completed development and validation of our coupled surface-subsurface flow and transport modeling workflow, and demonstrated its applicability to a large (10-km) segment of the Hanford Reach with transient simulations over a three-year period (2013-2015). To our knowledge, this is the most highly-resolved and

largest coupled transient surface-subsurface simulation ever performed, and its successful implementation is essential to mechanistic evaluation of central hypotheses related to the role of hydromorphology, hydrogeology, and dynamic river flows in controlling HEFs and biogeochemistry in large managed rivers. River hydrodynamics were simulated using the open source OpenFOAM code, applied at high resolution (10 m horizontally, 1 m vertically) using LIDAR-based bathymetry as input. Boundary conditions were provided from 1D simulation outputs from the PNNL code MASS1, previously calibrated for the Hanford Reach over the historical flow period. The 3D model was applied to a ~20 km segment of the Hanford Reach spanning a large meander (the "Horn") and the 100F and 100H areas (the focus of expanded SFA field instrumentation and research in FY19). Field observations of water surface elevation (WSEL) time series [*Niehus et al.*, 2014] were used to calibrate and validate the model. The primary calibration parameter represents riverbed boundary roughness, and we found that division of the 20 km domain into eight subdomains enabled accurate representation of observed WSELs. To minimize artifacts associated with upstream and downstream boundary conditions, the central 10-km section of the domain was extracted for subsequent analyses. Transient pressures at the riverbed output from OpenFOAM were passed to PFLOTRAN as boundary conditions to drive subsurface flow simulations. 3D groundwater flow velocities were simulated in a 6-km square domain (100 m thick in the vertical dimension) encompassing the 10-km river domain. Boundary conditions for the subsurface domain were imposed from outputs of reach-scale PFLOTRAN simulations generated by RC-A [*Shuai et al.*, 2019], and geologic property distributions from the reach-scale model were also employed at the local scale. The particle-tracking code developed by RC-A was employed to trace imaginary particles of water starting at the riverbed and moving through the subsurface environment, most of which eventually return back to the river (Figure 6 [left]). By tracing many such particles, we were able to generate residence time distributions (RTDs) and flux magnitudes of HEFs over the 10-km river segment. We combined the particle-based RTD outputs with maps of hydromorphic units (HUs) developed in FY18 to determine the relationship between HUs and RTDs under dynamic flow conditions. As shown in Figure 6 [right], we found that there are two characteristic groups of RTDs, one associated with HU classes "glide" and "riffle", and the other associated with the remaining five HU types. All RTDs exhibited multimodal patterns that could be represented as the sum of three Gaussian distributions.

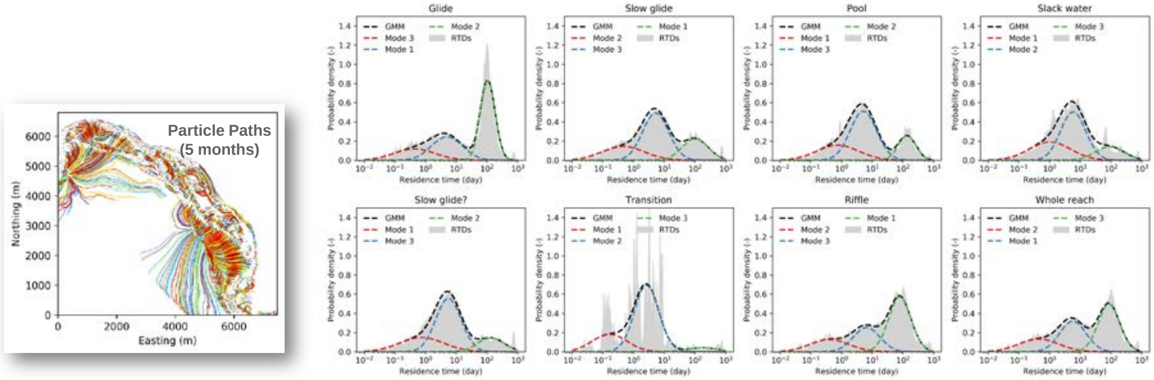

Figure 6 Left: Simulated particle paths within the 6x6-km domain, based on coupled surface-subsurface simulation results. Right: Computed residence time distributions (grey histograms) for particles starting on each of seven hydromorphic unit (HU) types, and for the entire domain. Dashed curves represent fitted Gaussian sub-modes.

These results provide preliminary confirmation of our key hypothesis that HU classes exhibit characteristic RTDs. The model outputs are currently being subjected to more detailed analysis using machine learning methods to identify additional factors that control RTDs and HEFs. One such factor is heterogeneity in riverbed material properties. We performed PFLOTRAN simulations using both homogeneous and heterogeneous riverbed properties, with the heterogeneous properties being assigned based on riverine facies maps -- see highlight below and [*Hou et al.*, 2019] -- and found that the heterogeneous properties significantly modified the RTDs and shifted residence times toward bimodal distributions with shorter travel paths that have greater influence on nutrient processing. Although the RTD shapes changed relative to the homogeneous base case, they retained similar relationships to HUs, again falling into two groups of characteristic shapes. This finding quantifies the important role of heterogeneous riverbed properties, suggests that riverbed heterogeneity significantly enhances nutrient uptake, and highlights the value of our facies mapping approach.

Publication Highlight: Riverbed heterogeneity maps inform PFLOTRAN simulations of HEFs

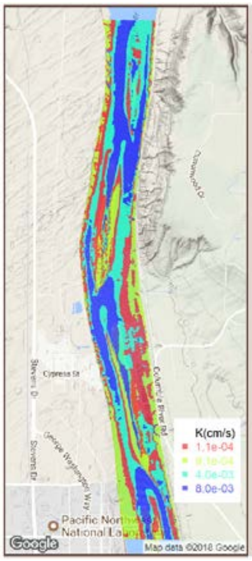

Figure 7 Hydraulic conductivity map over a 7-km river segment.

A novel approach to map riverbed properties over large spatial extents at high resolution was published in the journal *Hydrological Processes*. The methodology combines 2D river hydrodynamic model outputs with river bathymetry data to define riverine facies – classes of riverbed sediments with characteristic property distributions. Properties of interest include hydraulic conductivity and sediment texture. The method was applied to prescribe spatially heterogeneous conductance values that are currently being used as input for PFLOTRAN simulations in RC-B and RC-A. As described above, these heterogeneous properties led to significant changes in simulated RTDs (relative to a homogenous base case), specifically increasing the prevalence of short residence times that are typically associated with high nutrient uptake potential. Figure 7 shows a map of riverbed hydraulic conductivity based on the facies map over a 7-km section of river near the 300 Area; the method has been applied to the entire 70-km Hanford Reach and results are being used to study impacts of riverbed heterogeneity at local (RC-B) and reach RC-C) scales.

Reference: Hou, Z, T. D. Scheibe, C. J. Murray, W. A. Perkins, E. V. Arntzen, H. Ren, R. D. Mackley, and M. C. Richmond (2019) Identification and mapping of riverbed sediment facies in the Columbia River through integration of field observations and numerical simulations, *Hydrological Processes*, **33**, 1245-1259, doi: 10.1002/hyp.13396.

(2) Model-directed observational networks (ModEx): Results of RC-B mechanistic models were used to guide placement of new instrumentation and geophysical studies in the 100-F area by RC-C during the February 2019 field campaign. Maps of zones of predicted upwelling and downwelling were combined with HU maps and areas of cultural and ecological access restriction to identify candidate sites for installation of flux tools and thermal rods. Primary and alternate sites were identified, and locations were adjusted in real time based on field conditions through interactions between RC-C and RC-B team members. This effort was presented at the 2019 PI meeting as a "ModEx success story."

(3) New reaction networks represent biogeochemical impacts of microbial community composition and carbon character: Inspired by data generated through the WHONDRS network (see RC-C), we are developing new multi-omics-informed reaction networks to quantify the impacts of organic carbon character and microbial community composition on river corridor biogeochemistry. These new reaction networks will be integrated into PFLOTRAN for use in reactive transport simulations at hydromorphic feature scale (this Campaign) and at reach scale (RC-A). This work (being performed in close collaboration with KBase) has developed a novel pipeline that can construct metabolic networks based on the combination of metagenomic and metabolomic data, and will significantly advance predictive capabilities of reactive transport models [*Meile and Scheibe*, 2019]. Under SBIR funding, Roelof Versteeg is developing and testing workflows for automated solution of metabolic reaction networks generated by our pipeline using Flux Balance Analysis, and integration of those solutions into PFLOTRAN. This exciting development opens up the possibility of expanding WHONDRS into the modeling sphere through consistent generation of reactive transport simulations across a wide range of river systems using metabolomic and metagenomics data already collected by WHONDRS. Such a capability will provide major new insights into commonalities and differences in river corridor biogeochemistry between systems, and will support identification of the features of those systems that determine biogeochemical function.

Plans for FY20

As field observations become available from instrumentation recently installed at 100-F/H by RC-C, we will use those data to test, validate, and further refine our simulations. We will complete and publish the results of extensive machine learning analyses applied to coupled surface-subsurface simulation outputs, which will provide the basis to generate reduced-order representations to be applied at reach and larger scales. Reduced-order model formulation and parameterization will be done in coordination with RC-A, which is building reduced-order models into watershed-scale simulations. We will perform additional simulations using the coupled model workflow to explore impacts of formation-scale heterogeneity, and we will initiate PFLOTRAN reactive transport simulations to develop mechanistic understanding of impacts of HEFs and RTDs on nutrient uptake, and to further support reduced-order model development. We will continue to advance new multi-omics-informed reaction network models and utilize these models both to inform mechanistic-scale models of our system and to study cross-system transferability through a pilot modeling component of WHONDRS (with RC-C).

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.

FY19 Research Targets

FY19 Science Plan Milestone: Use data from automated hydrobiogeochemical monitoring and reactive tracer injections to feedback with RC-B in order to evaluate influences of variable discharge on HEFs and biogeochemical rates. Reveal processes governing DOC character and the follow-on impacts to biogeochemical function, and feedback with RC-B to include resulting process knowledge in reaction networks. Complete reach-scale organic carbon surveys to inform local- and reach-scale models.

Progress Brief for FY19

Research within and beyond the SFA continues to show that DOM chemistry has a strong influence on biogeochemical cycling in river corridors. In FY19, we focused on experiments, field observations, sensor development, and community engagement aimed at quantifying these controls and developing new approaches for modeling DOM-based reactions used in RC-A and RC-B.

(1) Integrated studies of DOM chemistry impacts on river corridor biogeochemistry: Reactive transport models do not currently consider chemical properties of DOM, indicating a significant structural gap that limits our ability to predict integrated hydro-biogeochemical function. To enable the incorporation of DOM chemistry into reactive transport models, we have pursued integrated research to (1) characterize spatiotemporal patterns in DOM chemistry, (2) reveal mechanisms that underlie subsequent influences on river corridor biogeochemistry, and (3) develop new representations of DOM chemistry that can be incorporated into numerical models. A major piece of our efforts is the WHONDRS consortium that we are using to advance cross-system characterization of patterns in DOM chemistry and integrated hydro-biogeochemical function of river corridors. For additional details on WHONDRS, please see the associated sub-section below, under 'Collaborative Research Activities.' To further evaluate mechanisms underlying biogeochemical impacts of DOM chemistry, we paired laboratory experiments with new biogeochemical modeling approaches that account for thermodynamic and microbial regulation of respiration. Aerobic sediment slurries revealed that transitioning from C-limited to C-replete conditions was associated with a transition from thermodynamic regulation of respiration (Figure 8) to limitation by organic N. These results point to interactions among thermodynamics, C concentration, and organic N availability as key controls on respiration rates in river corridors. In addition, these results challenge classical theory that discounts the relevance of DOM thermodynamics under aerobic conditions. To better understand the contradiction between theory and experimental outcomes we developed a numerical model—in collaboration with RC-B—to investigate the biogeochemical role of DOM chemistry in aerobic environments. The model revealed that thermodynamically favorable DOM promotes mineralization of less favorable DOM. Model outcomes therefore provide additional support to the inference that thermodynamic properties of DOM influence biogeochemical rates under aerobic conditions. This suggests the need to reconsider classic theory and revise models accordingly. Our efforts associated with DOM chemistry are collectively providing the data, mechanistic knowledge, and theory to integrate DOM chemistry with hydrology to enhance predictive understanding of hydro-biogeochemical function in river corridors.

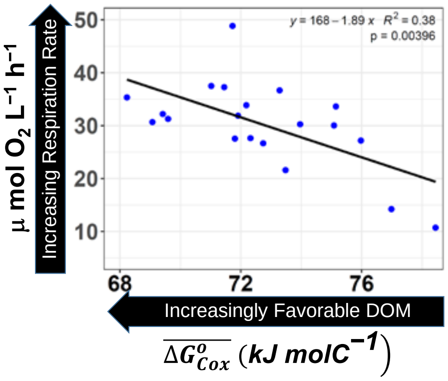

Figure 8 Respiration in hyporheic zone sediments increases with thermodynamic favorability of DOM. Such influences are not represented in state-of-the-art models.

Publication Highlight: Multi 'omics comparison reveals metabolome biochemistry, not microbiome composition or gene expression, corresponds to elevated biogeochemical function in the hyporheic zone: Biogeochemical hotspots are pervasive at terrestrial-aquatic interfaces, particularly within groundwater-surface water mixing zones (hyporheic zones), and they are critical to understanding spatiotemporal variation in biogeochemical cycling. We used multi 'omic comparisons of hotspots to low-activity sediments to gain mechanistic insight into hyporheic zone organic matter processing.We hypothesized that microbiome structure and function, as described by metagenomics and metaproteomics, would distinguish hotspots from low-activity sediments by shifting metabolism towards carbohydrate-utilizing pathways and elucidate discrete mechanisms governing organic matter processing in each location. We also expected these differences to be reflected in the metabolome, whereby hotspot carbon (C) pools and metabolite transformations therein would be enriched in sugar associated compounds. In contrast to expectations, we found pronounced phenotypic plasticity in the hyporheic zone microbiome that was denoted by similar microbiome structure, functional potential, and expression across sediments with dissimilar metabolic rates. Instead, diverse nitrogenous metabolites and biochemical transformations characterized hotspots. Metabolomes also corresponded more strongly to aerobic metabolism than bulk C or N content only (explaining 67% vs. 42% and 37% of variation respectively), and bulk C and N did not improve statistical models based on metabolome composition alone. These results point to organic nitrogen as a significant regulatory factor influencing hyporheic zone organic matter processing. Based on our findings, we propose incorporating knowledge of metabolic pathways associated with different chemical fractions of C pools into ecosystem models will enhance prediction accuracy.

Reference: Graham, E.B. et al. 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. https://doi.org/10.1016/j.scitotenv.2018.05.256

To further advance our mechanistic understanding we submitted a successful EMSL user proposal (*"Integrating thermodynamic and microbial mechanisms to understand coupled controls of carbon and nitrogen on hyporheic zone metabolism")*. We hired a post-doc (Swatantar Kumar) specializing in both environmental microbiology and stable isotope labelling approaches to lead the associated experiments. Kumar has worked closely with EMSL technology leads to decipher isotopic enrichment in metabolite profiles in preliminary experiments. A full scale experiment to trace sediment decomposition of 13C-labelled complex DOM (willow leaf) in the presence of simple organic C (glucose and glucosamine) with contrasting stoichiometries is planned for July 2019. This experient was designed in tandem with reactive transport models and will leverage EMSL technologies to couple the mechanisms of DOM decomposition across a range of respiration rates and DOM compositions. This line of inquiry will further scale to column-based experiments with real-time multiscale measurements (metabolomics and respiration rates), with a goal of in-situ experiments in FY20. Furthermore, given our leadership in environmental DOM analyses, we hosted a SCGF in summer 2018 (Garrett Rue). Using our analytical approaches, Rue was able to demonstrate linkages between C and P cycles in alpine lakes. To link DOM chemistry to influences of hydrologic and geochemical history, we conducted an initial study in the Hanford Reach using a combination of ion resin probes, respiration measurements, DOM chemistry analysis, microbial ‘omics, and field sensors. This is being done in collaboration with EMSL, and sample analysis is ongoing.

(2) Develop new understanding of coupled hydrologic and biogeochemical processes in the hyporheic zone through field experimentation and novel instrumentation linked to numerical models: To better inform coupled hydro-biogeochemical models of hyporheic zone function, we are pursuing in-situ tracer injections and developing novel tools and analytic techniques that enable simultaneous monitoring of dynamic fluxes and hyporheic zone respiration rates. Reactive and conservative tracers will be injected directly into the Hanford Reach riverbed, with a focus on elucidating aerobic respiration and N-cycling processes. This is being done in conjunction with our university collaborator, Bob Hall. We refer to the new tools as the ‘flux tool’ and the ‘optode-based oxygen sensor.’ The flux tool consists of a vertical array of sensors deployed into the riverbed. Its purpose is to measure hydrologic flux through riverbed sediments and the hyporheic zone. A novel aspect of the flux tool is that it can measure fluxes under both dynamic and steady-state conditions. Existing methods only work under steady state conditions and are not applicable to highly variable flow conditions in the Hanford Reach associated with dam operations. The flux tool is also likely to be very useful in tidally-impacted coastal systems that are never in steady state. The surface water hydrology of tidal systems is very similar to the Hanford Reach (i.e., regular sub-daily increases and decreases in river stage); no other technology exists to measure hydrologic flux

through riverbed sediments in such systems. Through WHONDRS we evaluated this possibility in a freshwater tidal portion of the Altamaha River, GA. Riverbed pressured gradients measured by the flux tool tracked surface water hydrology very closely. This provided an important and successful test of the technology outside the Hanford Reach.

The flux tool was originally built to measure 1-D (vertical) hydrologic flux. The sensors record time series of vertical gradients in pressure, temperature, fluid electrical conductivity, and bulk electrical conductivity. Collectively, these time series provide adequate information to estimate the vertical distribution of porosity and permeability using a companion high-performance hydrogeophysical joint inversion software. Initial field deployments have indicated significant lateral flow, in addition to vertical flow. Therefore, we have changed the field configuration to deploy three flux tools simultaneously, and we have modified the computational software to infer 3-D flow. This is a major step forward as no other technology can provide information on high-resolution 3-D hydrologic exchange flows. We currently have one set of 3-D flux tools deployed on Hanford Reach in the 100H area. The deployment location was informed by simulations performed under RC-B as described above, and resulting data will be used to evaluate model predictions of hydrologic flux. To further develop the flux tool technology we have contracted with the OpenS lab at Oregon State University to enhance streamlined deployment and data logging. The next generation of the 3-D flux tool will be used in additional locations in the Hanford Reach and in WHONDRS deployments in other river corridors. To complement the flux tool, we designed, built, and deployed additional sensor rods that measure vertically distributed temperature. Because these ‘thermal rods’ are far less expensive, we are evaluating the potential of using them in conjuction with the flux tool to infer hydrologic fluxes. To this end, we used RC-B model outputs to guide the deployment of 7 thermal rods around the 100H Area, across hydrogeomorphic classes (riffles, slow glides, and transitions) and across levels of predicted hydrologic flux. The deployments were also co-located with ground-based geophysical surveys led by RC-B to provide physical context and guide model refinements. Furthermore, we have paid careful attention to data structure and archiving to streamline modeling of these data by RC-A and RC-B. The OpenS lab is designing another sensor rod that combines vertically distributed temperature and pressure measurements. These ‘temperature/pressure rods’ are meant to replace the flux tool following in-situ calibration. That is, once the 3-D flux tool system is deployed in-situ, the numerical model is calibrated for the studied system using data produced by the flux tool. The flux tool can then be removed and the ‘temperature/pressure’ rods installed. The calibrated model can then estimate hydrologic flux using only temperature and pressure gradients. Because the ‘temperature/pressure’ rods are much less expensive, they significantly enhance our ability to measure fluxes across multiple locations within and across river corridors. We are using the same concept and approach to quantify exchange at larger scales by integrating 3D time-lapse ERT imaging with flow and transport modeling to estimate the larger scale porosity and permeability distributions that govern exchange flows. This approach is being developed and demonstrated using data collected on the comprehensive array. Once the 3-D system is calibrated, we will be able to quantify 3-D exchange flows at larger scales using observations of river stage and inland water table measurements.

Understanding coupled hydro-biogeochemical processes requires knowledge of both reaction and transport timescales. The flux tool provides flow data, but existing methods for measuring in-situ HZ respiration are inadequate. To fully link hydrology and biogeochemistry, we have been developing a sensor to measure HZ oxygen concentrations at high spatial and temporal resolution. Previous work has shown limited success using off the shelf fiberoptic oxygen sensors combined with custom optode-coated tubes. We are pursuing that approach, while simultaneously developing a more robust and compact system with no moving parts to measure and log a linear profile of HZ oxygen concentration. We are currently testing the ‘optode-based oxygen sensor’ alongside the flux tool to gain integrated hydro-biogeochemical insights.

(3) The SFA strives to be a leader in open community science: Applying the philosophy and approach of WHONDRS, we are leading a global consortium of researchers in developing a new conceptualization of disturbance-based research. This effort takes a novel approach, whereby any researcher is able to contribute and paper development is entirely open and publicly available. The paper

has been widely advertised via Twitter and has yielded over 50 active collaborators with no prior relationship to the SBR program. In addition, we developed a number of new collaborations—and deepened existing collaborations—with university researchers associated with the most recent SBR FOA.

Plans for FY20

In FY20 Campaign C will continue to develop the flux tool and optode-based sensing systems as well as expand on existing WHONDRS efforts, potentially targeting a more spatially intensive network of collaborators across the Columbia River Basin. Campaign C will also continue to develop and maintain the sensor network distributed around the 100H Area, conduct any necessary follow-on studies associated with in-situ reactivec/conservative tracer injections, and work with Campaign B to design and conduct additional experiments focused on DOM chemistry and potentially the interaction between DOM chemistry and environmental history.

Publication Analysis

71 peer-reviewed journal articles and one peer-reviewed book chapter have been published or are in press during the current triennial period (2017, 2018, and 2019 to date - see Appendix A for a complete list). Over this period, the SFA published most frequently in two journals, *Water Resources Research* (14 papers) and *Environmental Science & Technology* (8 papers). These two journals are among the top-ranked by ISI 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 papers were published in 37 different journals, reflecting the diversity of SFA research and the wide audience reached by our publications. The SFA publishes in high-quality journals: Two publications are in DOE-designated high-impact journals (*Nature Communications* and *Nature Microbiology*), approximately half (49%) of the publications are in ISI-designated top ten journals in their respective fields, more than three-quarters (78%) are in first quartile journals, and nearly all (97%) are in journals with impact factors above the median in their field. The average impact factor of the journals for which data are available (weighted by the number of SFA papers published in each) is 4.49.

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.[1] The long-term vision of the SFA, closely aligned with this SBR program objective, 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 other watershed hydrobiogeochemical system component models to provide predictive understanding of watershed function. In the current Triennial Period (FY18-20) we are expanding our 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 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 to have initiated efforts to integrate that capability with larger-scale modeling systems such as E3SM and the National Water Model.

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[1] https://doesbr.org/documents/SBR_Brochure.pdf

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

FY19 is the second year of the current Triennial Period for which our research plan was reviewed in 2017. The plan is currently being implemented largely as written and no near-term major 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. The large body of observations being made through WHONDRS are revealing new system behaviors and identifing additional gaps in understanding. We have made key discoveries and model developments focused on the role of organic carbon character in hydrobiogeochemical processes, and are considering expansion of that focus into new areas such as the study of black carbon abundance and impacts. Reach- and local-scale modeling studies have demonstrated important impacts of HEFs on temperature in the hyporheic zone, which is a critical factor in ecosystem health, suggesting increased emphasis on that aspect of water quality in future studies. Several of our activities have incorporated aspects of machine learning, and we anticipate that our project will continue to increase our emphasis on the integration of data-driven and process-driven models to elucidate and predict system behaviors.

Collaborative Research Activities

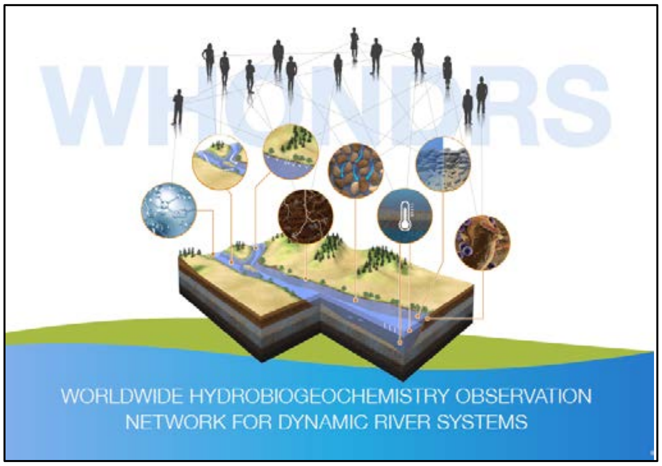
The SFA is dedicated to implementing principles of open, collaborative, integrated team science. We have made intentional and extensive efforts to increase our collaborative footprint over the past two years through a number of avenues including (1) direct-funded (by subcontract) collaborations to two other national labs, five universities, and the U.S. Geological Survey; (2) collaborative projects funded through SFA FOAs to university partners, with the SFA being either co-funded (8 projects) or unfunded (4 projects); and (3) collaborative projects funded through the SBIR program (5 projects). Lists of collaborative projects with co-PI names, institutions, and titles are provided in Appendix C.

SFA team members are also actively leading and involved in a number of community-level cross-cutting activities:

- Workshop Leadership: (1) Open Watershed Science Workshop: Co-PI James Stegen led the planning and execution of a BER workshop held in Bethesda MD on Jan. 28-29, 2019. (2) Integrated Hydro-Terrestrial Modeling Workshop: PI Tim Scheibe is organizing this interagency workshop to be held in Alexandria VA on Sept. 4-6, 2019; (3) The SFA will host the 2019 Watershed Community Workshop in Richland WA on Sept. 10-12, 2019.
- 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.
- ESS-Dive: The ESS-Dive team has visited PNNL twice to discuss opportunities and needs. A significant portion of the discussions focused around the SFA data archive approach and future needs. Based in part on these discussions, ESS-Dive has developed an interface that can be used to upload data from our 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.
- KBase: Campaign B Activity Lead Hyun-Seob Song is working closely with KBase staff (Chris Henry of ANL) to develop new workflows to integrate multi-omics data into microbial community reaction networks. These networks are then formulated into elemental reaction pathways that can be incorporated into reactive transport simulations using the PFLOTRAN reaction sandbox.
- IDEAS: Co-PI Xingyuan Chen is the PNNL lead for the IDEAS-Watershed collaborative project. Under this project the SFA will co-fund a post-doctoral associate that will work on developing community cyberinfrastructure, in part focused around the work with KBase described above.
- ExaSheds: Co-PI Xingyuan Chen is the PNNL lead for the ExaSheds pilot project, which is developing next-generation high-performance watershed modeling capabilities that will be integrated with and informed by artificial intelligence methodologies.

- Quarterly Community Teleconferences: We have hosted quarterly teleconferences, open to the scientific community, in which we share recent SFA advances and invite collaborators to present their research.

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 coupled hydrologic, biogeochemical, and microbial function, from local to global scales, within river corridors experiencing recurring, episodic, or chronic hydrologic perturbations. While our understanding of dynamic river corridors is increasing, there is still significant uncertainty in the hydrobiogeochemical impacts of hydrologic perturbations, 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 hydrologic perturbations, water quality, and the health of dynamic river corridors under future environmental conditions at regional, national, and global scales. The direction of WHONDRS has been guided by insights derived within the Hanford Reach of the Columbia River, our focal watershed test bed. WHONDRS provides data and knowledge that places those local insights in the context of river corridors distributed globally.



WHONDRS' distributed scientific approach is based on identifying critical scientific questions and providing targeted 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) to ensure consistent data products that use robust community data and metadata standards. WHONDRS is working with EMSL and ESS-DIVE to store all raw and processed data and metadata - which undergo rigorous quality assessment - in publicly accessible data archives. These efforts have generated two datasets published on ESS-DIVE [*J.C. Stegen et al.*, 2019; *J. C. Stegen et al.*, 2018], and 7 more are currently in the final quality assurance phase just prior to publishing. All data are published as soon as possible after they have been quality-checked so that the community can openly access and use the data for their work.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 have accumulated into a large compendium of data and knowledge, from which general principles can be derived.

WHONDRS is currently engaged in answering major, model-relevant scientific questions such as 1) is there a core metabolome across river water and riverbed sediments?, 2) what combination of environmental features explain variations in transient metabolomes?, 3) what are the relative contributions of ecosystem metabolomes and microbial communities in explaining variation in respiration rates of surface water and riverbed sediments?, and 4) how do surface hydrologic dynamics influence surface-subsurface hydrologic exchange across river corridors? WHONDRS is working towards these and other scientific questions by pursuing three primary efforts: 1) identification of surface water metabolites and their dynamics in response to river stage fluctuations (over 140 sampling kits distributed), 2) developing new sensor technology to estimate sediment porosity and the mass flux of water moving through the hyporheic zone as described above (Campaign C Progress), and 3) investigation of surface water and sediment metabolites, microbial communities, and geochemistry across the U.S., from Alaska to Puerto Rico (over 40 sites have agreed to sample; will occur August 2019).

WHONDRS also completed a sampling campaign in August 2018 that aimed to study diel cycling in seven global rivers with different drivers of stage variation (i.e., hydropower dam, glacial melt, wastewater effluent, evapotranspiration, tidal, groundwater pumping). For this study, sampling kits were sent to collaborators who then sampled surface water and pore water every three hours for 48 hours. These metabolomics efforts, using EMSL's Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FTICR-MS), 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.

Collaborator engagement is fundamental to WHONDRS' success and has continued to increase. Given strong community interest WHONDRS has needed to increase analysis throughput for FTICR-MS data. To date, WHONDRS is associated with over 1500 FTICR-MS samples run at EMSL. To accommodate this large number of samples WHONDRS collaborated with EMSL to compile an automated analysis pipeline. This pipeline has been provided to the community via the most recent WHONDRS dataset archived on ESS-DIVE (Stegen et al. 2019). To expand molecular analyses beyond FTICR-MS and provide a multi-omic resource to the community, WHONDRS is collaborating with a group of ten PIs on a very large (14 Tb) JGI CSP proposal, led by Kelly Wrighton. This CSP will support WHONDRS sampling efforts in August 2019 associated with a number of the science questions summarized above. In addition, the SFA has sub-contracted with Kelly Wrighton to handle all processing and analysis of microbial samples.

At its core, WHONDRS is committed to removing barriers and enabling the community. WHONDRS has worked to raise its profile to further encourage community participation and to help shift the community towards adoption of open, distributed science. For example, an editorial summarizing WHONDRS was published in mSystems [*J. C. Stegen and Goldman*, 2018], and WHONDRS was called out as an example of a distributed network enabling development of transferable knowledge [*Graham et al.*, 2019]. WHONDRS had a Town Hall, social event, several oral presentations, and an exhibit hall booth at the American Geophsyical Union (AGU) Fall Meeting in December 2018. The Town Hall included a demonstration of the GUI WHONDRS developed to allow anyone to rapidly explore within datasets and to parse the full dataset into subsets of interest, without the need for programming skills. ESS-DIVE also held a demonstration of their tools using WHONDRS data at the WHONDRS AGU exhibit booth. James Stegen was invited to give a WHONDRS briefing to BER in November 2018 and will give an invited talk about WHONDRS at the American Chemical Society in August 2019. WHONDRS was included as part of an AAAS session proposal for 2020 on the role of open science. The increasing visibility and output of WHONDRS contributed to it being called out at as a BER capability in the most recent SBR FOA for universities. In response, WHONDRS was included in multiple university proposals, including one TES proposal, two SBR proposals, one NSF proposal, and two Early Career proposals. WHONDRS was also a catalyst and key to development of the vision for the DOE Open Watersheds by Design workshop, for which James Stegen was co-lead. The vision emerging from that workshop was successfully presented to BERAC in April 2019. Upcoming efforts will begin to develop a citizen science component to WHONDRS through a STEM outreach program at PNNL.

APPENDIX A: PROJECT PUBLICATIONS

2019

Published:

Dai H., Chen X., Ye M., Song X., Hammond G., Hu B. X. and Zachara J. (2019) Using Bayesian networks for sensitivity analysis of complex biogeochemical models. *Water Resources Research*, 55; doi: 10.1029/2018WR023589

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APPENDIX B: LISTING OF COLLABORATIVE PROJECTS

Direct-Funded Collaborations – The SFA has directly funded the following external collaborations during the current triennial period:

- (2017-Current) Heping Liu, Washington State University – Install, maintain, and process data from eddy flux towers at multiple locations along the Hanford Reach for Campaign A.
- (2017-2019) Gautam Bisht and Bill Riley, Lawrence Berkeley National Laboratory – Collaborate with Campaign A on linking CLM with PFLOTRAN, and test performance with various interaction zone and climate scenarios.
- (2017-Current) Glenn Hammond, Sandia National Laboratory – Support PFLOTRAN development and implementation in Campaigns A and B, including incorporation of new reaction network models.
- (2017-2018) Eric Roden, University of Wisconsin – Collaborate with Campaign C to investigate carbon sources driving microbial activity in the subsurface interaction zone.
- (2017-Current) Jesus Gomez-Velez, Vanderbilt University – Apply the NEXSS model to our experimental system (Hanford Reach and Priest Rapids – Lower Columbia Watershed). Collaborate with Campaigns A and B to incorporate new mechanistic understanding into NEXSS and couple it with other watershed modules.
- (2019-Current) Kelly Wrighton, Colorado State University – Collaborate with Campaign C on microbial community analysis including metagenomics studies for WHONDRS.
- (2019-Current) Ty Ferre, University of Arizona – Collaborate with Campaign A to perform numerical studies employing data assimilation methods to optimize sensor configurations for estimation of hydrologic exchange fluxes.
- (2019-Current) Jeff Wiles, US Geological Survey – Install and maintain monitoring system for an irrigation return channel in the Hanford Reach and incorporate data into USGS water data system; see https://waterdata.usgs.gov/nwis/uv?site_no=12473503.

SBR-Funded University Collaborations – The SFA collaborates closely with several university-led projects funded by the SBR program:

Co-Funded Collaborators (PNNL receives limited supplemental funds under these projects):

- Tom Bianchi (Florida State University): The Influence of Microbial Priming Effects on the Hydro-bio-geochemistry in the Columbia River and its Tributary Confluences
- Bayani Cardenas (University of Texas Austin): Respiration in Hyporheic Zones: Advancing the Understanding of Coupled Transport and Microbial Biogeochemistry and their Representation in Open-source Mechanistic Models
- Tim Covino (Colorado State University): Persistent Effects of Forest Harvest on Dissolved Organic Matter Composition in Subsurface Hillslope Runoff
- Nick Engdahl (Washington State University): Transient cycling of nitrogen, organic carbon and oxygen within the free-flowing Columbia River corridor: Linking exposure time dependent biogeochemical reactions to river stage fluctuations
- Ricardo Gonzalez-Pinzon (University of New Mexico): Physical, Resource Supply, and Biological Controls on Nutrient Processing Along the River Continuum
- Robert Hall (University of Montana): Scaling hyporheic nitrogen cycling in large river alluvial aquifers
- George Karniadakis (Brown University): M&M: A Multi-Fidelity & Machine-Learning Approach to Model Hydrologic-Biogeochemical Processes in the Groundwater-Surface Water Interaction Zone

- Kelly Wrighton (Colorado State University): Methane and Nitrous Oxide Pore-Water Concentration and Flux at the Hyporheic Zone of a Large River

Unfunded Collaborations (PNNL supports these projects under SFA scope without separate funding):

- Michael Gooseff (University of Colorado): Water Management Impacts on Groundwater-River Water Exchanges
- Daniel Tartakovsky (Stanford University): Assimilation of Multiscale Data into Multifidelity Biogeochemical Models
- Adam Ward (University of Indiana): Coupled Investigation of Hyporheic Transport and Transformation Dynamics in Headwater Streams: Preliminary Findings and Experimental Design
- Ming Ye (Florida State University): Using Global Sensitivity Analysis to Identify Controlling Processes of Complex Systems

<u>SBIR-Funded Industrial Collaborations</u> – The SFA works with a number of small businesses to apply and test new technologies at our field and laboratory sites:

- Ruby Ghosh (OptiO2) – Probing Biogeochemical Processes with High-Resolution/Long-term Dissolved Oxygen Measurements
- Matt Fisher (IWT) - Integrated sensor network provides near real-time temporal and spatial measurements for capturing in situ parameters to characterize fate and transport of solutes in hydrobiogeochemical systems
- Yuhong Kang (NanoSonic) Integrated Nanomembrane based Chemical Field Effect Transistors (ChemFETs) for Groundwater Monitoring
- Keith Jameson (Amethyst Research) – Greenhouse Gas Imaging and Monitoring Camera
- Scott Burge (Burge Environmental, Inc.) Automated Monitoring of Subsurface Microbial Metabolism with Graphite Electrodes

APPENDIX C: REFERENCES CITED

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