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Pacific Northwest National Laboratory SFA Annual Report

River Corridor Hydrobiogeochemistry from Reaction to Basin Scale

June 2022

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PNNL River Corridor Scientific Focus Area Annual Report FY2022

River Corridor Hydrobiogeochemistry from Reaction to Basin Scale

2022 Annual Report

June 30, 2022

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I. PROGRAM OVERVIEW

The Pacific Northwest National Laboratory (PNNL) River Corridor Science Focus Area (SFA) is transforming understanding of spatial and temporal dynamics in river corridor hydrobiogeochemistry from reaction to watershed and basin scales, enabling mechanistic representation of river corridor processes and their responses to disturbances in multiscale models of integrated hydrobiogeochemical function.

Our research is focused on understanding the controls on spatial and temporal variations in river corridor hydrobiogeochemistry, hydrobiogeochemical responses to wildfires and other disturbances, and representation of river corridor hydrobiogeochemistry in numerical models from reaction to basin scales. The project's goals are aligned with the objective of DOE's Office of Biological and Environmental Research (BER) to improve scientific understanding and prediction of the function of natural and managed watersheds and their responses to disturbances.

Our long-term vision is to mechanistically link the impacts of disturbance on hydrologic exchange flows (HEFs, the exchange of water between surface and subsurface environments in river corridors), molecular processes, and biogeochemistry to watershed function across CONUS basins. This vision is being achieved through distributed, basin-scale science pursued via extensive collaboration with the research community following ICON-FAIR principles (DOE, 2019). These principles focus on doing science by-design that **I**ntegrates physical, chemical, and biological processes, is **C**oordinated via consistent methods from field to lab to analysis, uses **O**pen science methods such as making data FAIR, and is **N**etworked with the community to enable distributed data generation and modeling that are mutually beneficial to all. Our hypothesis-driven approach advances transferable understanding of coupled hydrobiogeochemical processes through integrated multiscale experiments, observations, and modeling. Enabling mechanistic representation of river corridor processes from reaction to watershed and basin scales will provide a foundation for developing the next generation of watershed models with enhanced predictive capacity to inform watershed management strategies aimed at solving the nation's environmental challenges in the face of extreme disturbances.

Progress toward this vision is achieved through four Research Campaigns (RCs) integrated through a Multiscale ModEx approach as shown in Figure 1, in keeping with the concept of iterative model-driven experimentation and observation. 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 four campaigns to address high-level project objectives.

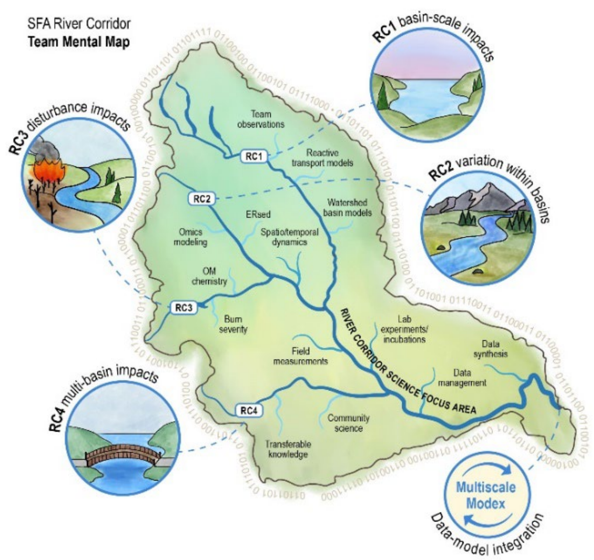

Figure 1. The "Team Mental Map" of the River Corridor SFA, in which Research Campaigns (RCs) are represented as major rivers in the Yakima River Basin (YRB), and characteristic activities are denoted as sub-catchments. Multiscale Modex is an iterative data-model learning loop in which models and experiments across scales are co-designed to test central hypotheses and develop predictive understanding.

- The *Cumulative Effects Campaign* (RC-1) aims to reveal the cumulative effects of river corridor processes and their appropriate representations in watershed- and basin-scale models.
- The *HBGC Variability Campaign* (RC-2) aims to elucidate interactions among hydrologic and molecular processes that control the cycling of nutrients (N, P), dissolved organic

matter (DOM), and inorganic contaminants (e.g., NO_3^-) in river corridors from reaction to basin scales.

- The *Watershed Disturbances Campaign* (RC-3) aims to reveal the mechanisms by which wildfires impact biogeochemical cycling in river corridors from reaction to basin scale.
- The *Multi-Basin Studies Campaign* (RC-4) aims to provide transferable principles that integrate DOM chemistry, microbial gene expression, biogeochemical function, and disturbance by combining existing global-scale data with Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems (WHONDRS)-based data generation and numerical modeling distributed across CONUS basins.

II. KEY SCIENTIFIC OBJECTIVES

In keeping with the vision outlined above, we have expanded both the physical scale and complexity of our research while maintaining our focus on the study of HEFs, DOM chemistry, microbial activity, and associated biogeochemical processes in the river corridor and their cumulative impacts at watershed and basin scales. Our long-term objective is to expand the scope of our study to the scale of the full Columbia River Basin (CRB) encompassing more than 460,000 km of perennial streams in an area of 670,000 km^2 and to extend the transferability of our science by studying multiple basins across the CONUS. Going to larger scales provides new opportunities to study broadly distributed disturbances and their impacts across diverse environmental conditions. Our work focuses on impacts of wildfire and precipitation, while spanning gradients in climate, vegetation, land use, and other key watershed features. As an intermediate step toward this long-term objective, in FY21-22 we have focused on study of the Yakima River Basin (YRB), a major sub-basin of the CRB in which there exists a wide range of stream orders and physiographic watershed settings, allowing us to generalize site-specific findings from our previous studies to have broad applicability. Our research is structured around the scientific grand challenge defined below.

Scientific Grand Challenge: Understand and quantify processes governing the cumulative effects of HEFs, DOM chemistry, microbial activity, and disturbances on river corridor hydrobiogeochemical functions at watershed to basin scales.

Dynamic HEFs are a primary driver of river corridor biogeochemistry, which is highly sensitive to DOM chemistry and microbial activity (e.g., expressed metabolic pathways). Disturbances such as wildfire and extreme precipitation interact to create feedbacks among physical and biogeochemical processes. These concepts motivate both fundamental process studies and the development/implementation of a multiscale modeling framework, and lead to the following SFA-level science questions that guide our research plan:

Overarching Science Questions:

1. How do HEFs, DOM chemistry, microbial activity, and disturbances interactively influence river corridor hydrobiogeochemical function from reaction to basin scales?
2. How can mechanisms that govern river corridor hydrobiogeochemistry be efficiently and sufficiently represented in integrated land surface models at scales relevant to regional and national water challenges?

III. PROGRAM STRUCTURE

The PNNL SBR-SFA is led by a Principal Investigator (PI, Tim Scheibe) and two Co-PIs (Xingyuan Chen and James Stegen) (Figure 2). In his role as Director of Program Development for PNNL's Earth and Biological Sciences Directorate, Scheibe also serves as the primary point-of-contact with the DOE-BER. The SFA is organized around four RCs (Figure 1), each of which is led or co-led by one of the three PIs. An early-career staff member, Allison Myers-Pigg, is co-leading RC-3 with mentorship from PI Scheibe, with the expectation of her development into a co-PI position over time. Each RC comprises two to three major activities; each activity is organized into several Sub-Activities. The Multiscale ModEx (MM) cross-cutting activity serves an integrating role to ensure that observational, experimental, and modeling research are highly coordinated. Activity Leads are responsible for coordinating research within each activity and are members of the SFA Leadership Team. Other key staff have responsibilities within one or more activities or sub-activities and contributing staff (including funded collaborators) are disciplinary experts that lead or contribute to one or more RCs. 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.

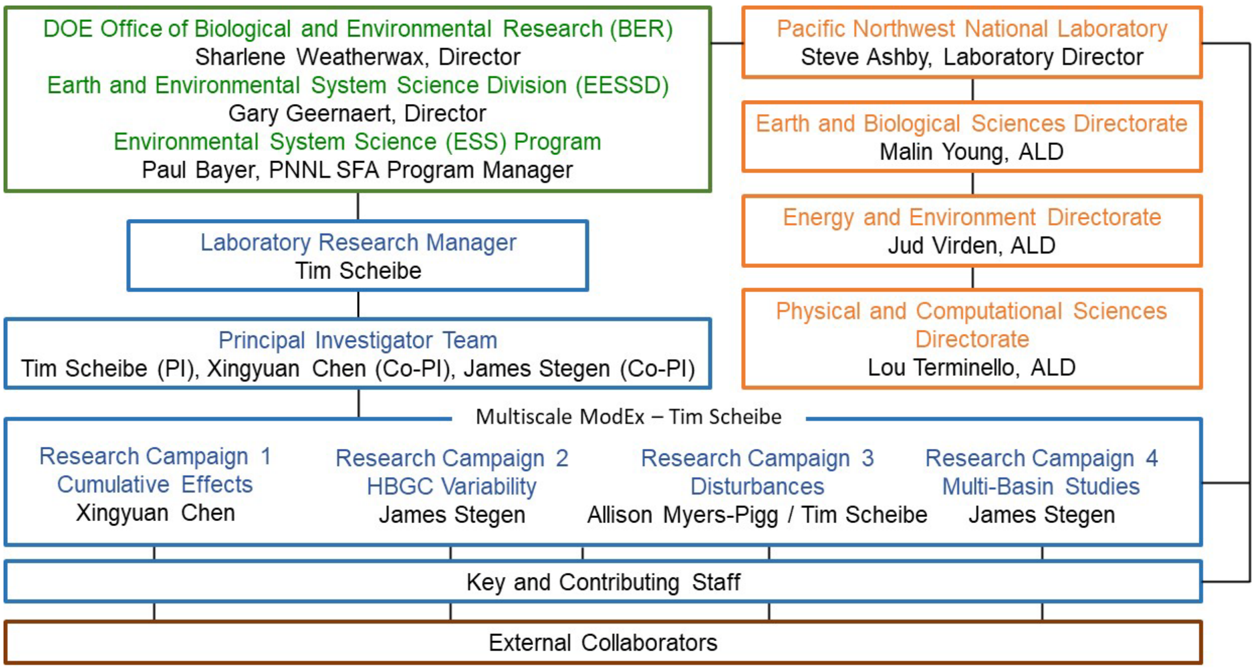

Figure 2. PNNL River Corridor SFA organizational structure.

Our management philosophy and process are 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 collaborative environments including Microsoft Teams (virtual meetings, file sharing, persistent chat), Atlassian Confluence (wiki), AirTable (task tracking), GatherTown (virtual workspace), and others. We are actively learning and applying principles of the Science of Team Science (SciTS) (NRC, 2015) to enhance transdisciplinary integration and teaming within the project and with external collaborators. For example, Figure 1 is a representation of the SFA "Team Mental Map" - a graphical representation of the mental model of the research objectives and collaborative structure shared by team members (Cannon-Bowers et al., 1993). Research in the SciTS field has shown that shared mental models enhance the effectiveness of science teams and other larger groups. Figure 1 was developed based on input from all team members and discussion of individuals' mental models of the project and is used in many contexts to communicate the overall project objectives and approach.

IV. PERFORMANCE MILESTONES AND METRICS

Review of Scientific Progress Toward Program Objectives and Milestones

Research Campaign 1 (RC-1): Cumulative Effects

Overall Objectives: *The Cumulative Effects Campaign aims to reveal the cumulative effects of river corridor processes and their appropriate representations in watershed- and basin-scale models.*

- Quantify baseline cumulative effects: Quantify the cumulative effects of river corridor HEFs, DOM chemistry, and microbial activity on watershed and basin biogeochemical cycling, water quality (including temperature), contaminant mobility, and land surface fluxes. Use reaction network models and rate kinetics developed from lab and field studies in RC-2 to inform river corridor reactive transport model.
- Quantify cumulative effects of disturbances: Reveal the cumulative impacts of wildfire and precipitation on watershed- to basin-scale hydrobiogeochemical functions of river corridors. Leverage new reaction networks and kinetics, focusing on the effects of wildfire-affected DOM chemistry on river corridor metabolism, developed in RC-3 in coordination with RC-2.
- Guide field and lab experiments: Provide basin-scale river corridor model outputs of biogeochemical hot spots and hot moments to focus field and laboratory experiments of RC-2 and RC-3 in locations and time windows that are most effective at reducing uncertainties in watershed model predictions.

Key Contributions of this Research Campaign to the SFA: RC-1 is integrating numerical models developed at multiple scales with distributed monitoring in other RCs across the YRB to advance predictive understanding of emergent system behaviors arising from complex hydrobiogeochemical interactions. We are building a watershed- to basin-scale river corridor model that links dynamic flow processes with variable temperatures and reaction kinetics (informed by molecular properties) to investigate water, energy, and mass fluxes across the river-groundwater interface. This model will be used to further quantify the cumulative impacts of HEFs, molecular properties, and disturbances on the watershed- and basin-scale biogeochemical cycling of key nutrients (C, N, P) and inorganic contaminants (e.g., NO_3^-).

FY22 Science Plan Milestone: Incorporate spatially variable reaction networks informed by molecular properties/processes and parameters from RC-2. Run paired watershed analyses for evaluating impacts of wildfire disturbances on river corridor biogeochemistry and stream temperature. Set up ATS and WRF-hydro models at representative watersheds, compare with CLM-PFLOTRAN in partnership with IDEAS-Watersheds. Design and implement modular watershed models with River Corridor components (partnership with IDEAS-Watersheds).

Note: We have adjusted our plan this year to focus more on ATS-PFLOTRAN simulations because we successfully compared ATS with National Water Model reanalysis data (equivalent to WRF-Hydro simulations) at American River Watershed in FY21, and CLM-PFLOTRAN will be replaced by ELM-ATS-PFLOTRAN in the next 1-2 years after this coupling is completed on the COMPASS project.

Progress Brief for FY22

Linking FTICR-MS Data with Reactive Transport Modeling in PFLOTRAN: Through collaboration with IDEAS-Watersheds, we have combined the KBase pipeline that digests FTICR-MS data to produce a respiration reaction expression with a PFLOTRAN reactive transport modeling workflow to seamlessly link the processing steps from reading in raw FTICR data, digesting it down to the appropriate reaction networks, and then running the reactive transport simulation in batch and 1-D column setup and analyzing results. This streamlined workflow will allow us to build spatially varying biogeochemical reaction networks from spatially distributed FTICR-MS measurements obtained by RC-2 and integrate them within watershed hydrobiogeochemical models. PFLOTRAN has been successfully containerized and can now be run through a Docker container and executed using an interactive, web-based Jupyter Notebook. This containerized version allows newer users to access the powerful reactive transport capabilities of PFLOTRAN regardless of their programming background and/or computer system and to gain an improved understanding of an experimental system.

Implementing NEXSS in the Yakima River Basin: The Vanderbilt team developed *pynexss*, a new Python implementation of the Networks with Exchange and Subsurface Storage (NEXSS) model with methods for preprocessing, geomorphological characterization, and estimating hyporheic exchange fluxes and residence times. The new implementation of NEXSS recognizes the uncertain nature of the input parameters and parameterizations at the core of NEXSS and facilitates quantification of uncertainty in hydraulic geometry, river discharge, and grain size using a Monte Carlo approach. The new NEXSS implementation is being tested in the YRB.

Integrated watershed HBGC modeling: Using a calibrated ATS model for the American River watershed (ARW) within the YRB, we investigated the impact of riverbed properties, including riverbed permeability, thickness, and width (defined as the finest resolution of the mesh), on surface-subsurface water exchange fluxes under different flow conditions. While discharge at the watershed outlet is not sensitive to changes in riverbed properties, exchange fluxes across the riverbed are heavily influenced by the riverbed properties. Fine mesh resolution around the river network was found to be critical for capturing the magnitude of exchange fluxes in small river segments. A lack of riverbed bathymetry data can contribute to uncertainty in biogeochemical cycling within river corridors. We are currently working on adding the denitrification reaction network into the integrated hydrologic model to quantify the amount of carbon and nitrogen transformed in the river corridors of the ARW and compare with SWAT-MRMT based estimations.

Impact of wildfire on hydrologic processes in the Yakima River Basin using the SWAT model: We used the Soil Water Assessment Tool (SWAT) model to assess the impact of fire-induced landcover change on hydrologic changes in YRB, where fires have been the driver of the land cover change. Our modeling analysis is focused on three large fires in 2012, 2013 and 2017. We built paired SWAT models using pre- and post-fire land cover data (NLCD) to allow the comparison between pre-fire and post-fire conditions. Comparison between the pre- and post-fire streamflow from the paired models shows that fire events increase peak flow and decrease baseflows in the watersheds. The increase in peak flows is found to be a combined effect of increased surface runoff and decreased ET, while decreased baseflows are associated with decreased soil water storage due to decreased infiltration. Such impacts are found to last for multiple years due to slow vegetation recovery, especially in the dry areas. Remotely sensed MODIS leaf area index product confirmed slow vegetation recovery rates in the fire-impacted areas within YRB.

Knowledge-guided machine learning for parameter estimation: We performed ATS calibration of 14 parameters in the ARW using a knowledge-informed deep learning technique developed by ExaSheds. A specific goal is to understand the interplay among multivariate observations of streamflow (Q), evapotranspiration (ET), and snow cover (SC) in model calibration in this snow-dominated area. A mutual information (MI)-based global sensitivity analysis (GSA) using 623 realizations showed that SC is sensitive to parameters related to snow melting, ET is mostly sensitive to Priestley-Taylor coefficients, and Q is mostly sensitive to the permeability of dominant soil types and geological layers, manning's coefficient and two snow melting parameters. Based on the GSA result, neural networks wer developed to estimate each parameter from the corresponding informative response variables that share non-zero MI with the parameter. We built the neural networks using uni-/bi-/tri-variate responses (Q, ET and SC) as input to test their individual and joint contribution to estimating different parameters, and consequently on the estimated parameters in capturing these responses over time. While use of all three types of observations yields the best overall performance, we also found that remotely sensed ET data products can be an effective alternative to Q in estimating watershed model parameters in ungauged watersheds.

Flux Tower Installation within YRB: The Washington State University (WSU) team installed two flux towers in YRB, one within the Evans Canyon fire scar and the other outside the fire scar. Each flux tower includes one eddy covariance system that consists of a sonic anemometer and an infrared CO2/H2O gas analyzer. The eddy covariance system provides fluxes of momentum, sensible heat, latent heat, and CO2. Besides the eddy covariance flux measurements at each site, there are a suite of measurements of microclimate variables. A four-component net radiometer is deployed to measure incoming shortwave radiation, reflected shortwave radiation, incoming longwave radiation, and outgoing longwave radiation. A temperature and humidity probe is used to measure air temperature and relative humidity. A rain gauge is used to measure 30-min total precipitation rate. Soil temperature and moisture as well as soil heat flux are measured at each site. The 10-Hz time-series data and the 30-min mean data are automatically transferred through Verizon wireless network to a server at WSU in a real-time manner. These two flux towers have been collecting data since April 2022.

Publication Highlight: Using Ensemble Data Assimilation to Estimate Transient Hydrologic Exchange Flow under Highly Dynamic Flow Conditions - Quantifying dynamic HEFs within river corridors that experience high-frequency flow variations caused by dam regulations is important for understanding the biogeochemical processes at the river water and groundwater interfaces. Heat has been widely used as a tracer to infer steady-state flow velocities through analytical solutions of heat transport defined by the diurnal temperature signals. Under sub-daily dynamic flow conditions, however, such analytical solutions are not applicable due to the violation of their fundamental assumptions. In this study, we developed a data assimilation--based approach to estimate the sub-daily flux under highly dynamic flow conditions using multi-depth temperature observations at a five-minute resolution. If the hydraulic gradient is measured, Darcy's law was used to calculate the flux with permeability estimated from temperature responses below the riverbed. Otherwise, flux was estimated directly by assimilating multi-depth temperature data at one- or two-hour time intervals assuming one-dimensional flow and heat transport governing equation. By comparing estimated fluxes with model-generated synthetic truth (Figure 3), we demonstrated that both schemes have robust performance in estimating fluxes under highly dynamic flow conditions. This data assimilation-based flux estimation method was able to capture the vertical sub-daily fluxes using multi-depth high-resolution temperature data alone, even in the presence of multi-dimensional flow. This approach has been successfully applied to real field temperature data collected at the Hanford site, which experiences highly dynamic HEFs. Our study shows the promise of adopting distributed 1-D temperature monitoring to capture spatial and temporal exchange dynamics in river corridors at watershed and larger scales.

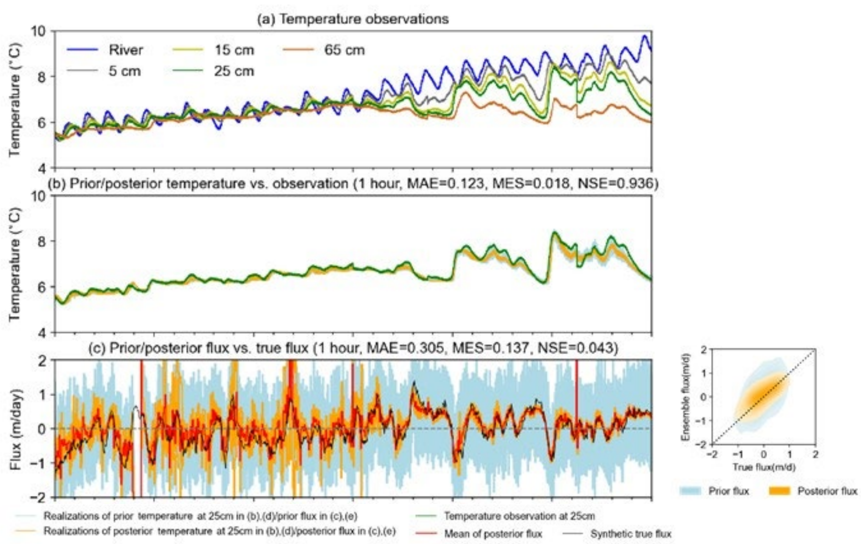

Figure 3 Evaluation of flux estimation performance using synthetic temperature profile observations generated from a 3-D model. We explored one- and two-hour assimilation time intervals; thermal conductivity and porosity are assumed known. (a) Synthetic temperature observations from the 3-D model. (b) Prior/posterior estimates of temperature time series (25 cm depth) using a one-hour assimilation time interval vs. corresponding synthetic temperature observations from the 3-D model; (c) Prior/posterior estimates of flux time series using a one-hour assimilation time interval vs. synthetic true fluxes from the 3-D model.

Reference: Chen, K., Chen, X., Song, X., Briggs, M. A., Jiang, P., Shuai, P., et al. (2022). Using ensemble data assimilation to estimate transient hydrologic exchange flow under highly dynamic flow conditions. *Water Resources Research*, 58, e2021WR030735. https://doi.org/10.1029/2021WR030735

Plans for FY23

In FY23, we will focus on 1) develop ATS-PFLOTRAN coupled models by incorporating heat transport and biogeochemical reactions for selected watersheds within YRB; (2) we will derive reaction networks in fire-impacted watersheds (collaborating with RC-3) and incorporate that into SWAT-MRMT model and ATS-PFLOTRAN model to investigate the impacts of fire on the HBGC regimes in river corridors; (3) examine the variations in reaction mechanisms across YRB using distributed molecular characterization performed by RC-2 and incorporate this variability into watershed HBGC models; (4)

use RC-2 sampling and monitoring data to evaluate and calibrate SWAT and ATS-PFLOTRAN models in YRB.

<u>Research Campaign 2 (RC-2): Hydrobiogeochemical Variability</u>

Overall Objectives: The HBGC Variability Campaign aims to elucidate interactions among hydrologic and molecular processes that control the cycling of nutrients (N, P), DOM, and inorganic contaminants (e.g., NO 3−) in river corridors from reaction to basin scales.

- <u>Identify important places/times</u>: Use NEXSS and SPARROW predictions (existing and from RC-1.1) to guide placement of in situ sensors to span a range of predicted respiration contributions of sediment-associated microbes (ERsed), relative to those in surface water. Use to identify where and when ERsed is disproportionately high.
- <u>Compare to predictions</u>: Compare field-estimated ERsed to NEXSS predictions and use outcomes to inform structure of and parameterize basin-scale models in RC-1.1.
- <u>Characterize variation</u>: Use field surveys across reaches that differ in ERsed to characterize longitudinal and seasonal variation in DOM chemistry, microbial gene expression, and nutrient concentrations in surface and pore water.
- <u>Inform models</u>: Use field survey data to inform 1-D reactive transport models that predict biogeochemical rates using explicit representation of DOM chemistry, microbial gene expression, and nutrient concentrations.
- <u>Understand consequences</u>: Use RC-1 models and field surveys to guide lab experiments to reveal influences of DOM chemistry, microbial gene expression, and nutrient concentrations on biogeochemical rates predicted by reactive transport models.
- <u>Refine models</u>: Use experimental outcomes to test and refine substrate/microbe-explicit reaction network models, use these models to evaluate impacts of PyOM in collaboration with RC-3, and integrate them into reactive transport models in collaboration with inform RC-1.

Key Contributions of this Research Campaign to the SFA: The SFA is designed to increase predictive understanding of the variations in river corridor hyrdobiogeochemical processes across stream orders as well as other climatic, ecological, and geographic settings. RC-2 has started to elucidate interactions among hydrologic and molecular processes that control the cycling of nutrients (N, P), DOM, and inorganic contaminants (e.g., NO3−) in river corridors by initiating a series of field-based sampling and monitoring campaigns across the YRB. As these campaigns generate data sets spanning both long periods of time and a broad variety of geographic settings, they provide the basis for both exploring the mechanistic linkages between process and setting, as well as iteration with numerical models to improve predictive ability.

FY22 Science Plan Milestone: Deploy sensors across low to high order reaches predicted to span a continuum of sediment contributions to system respiration. Compare outcomes to existing model predictions. Work with RC-1 to understand how deviations from model predictions inform need for additional process resolution in basin-scale models. Work with RC-3 to use outcomes to inform disturbance-focused field campaigns.

Progress Brief for FY22: Our activities in FY22 are focused on analysis of samples and data generated in FY21, providing stream chemistry data to RC-1, maintaining long-term monitoring of stream chemistry across sites in the YRB, leading a large cross-SFA field effort in the YRB designed as a spatial snapshot, further developing auto-chamber technology for stream metabolism quantification, and continuing to lay the logistic groundwork (e.g., permitting) for long-term hydrobiogeochemical field efforts in the YRB.

Large-scale field studies: As in FY21, RC-2's role in the RCSFA continues to be centered around a pair of large-scale field efforts in YRB. One campaign is designed to cover a smaller number of sites over an extended time period (the temporal study), while the other is designed to cover a large range of field sites over a brief period of time (the spatial study). The temporal study has continued in FY22 with relatively few modifications, and has become a mature and routine monitoring effort that is generating data needed by RC-1 models and that enable evaluation of spatiotemporal basin-scale science questions. The temporal study is focused principally on stream chemistry, and parameters/analytes were selected based on close coordination with RC1 to ensure the data meet their modeling needs. The six spatial locations of the temporal study were selected to span stream orders and to be co-located with stream gauges run by other agencies (i.e., USGS and Bureau of Reclamation). A second instance of the spatial study will be carried out in the summer/fall of FY22, with significant modifications relative to the spatial study of FY21, as detailed below.

Spatial variability of HBGC processes: The FY22 spatial study is led by RC-2 but has been co-developed with researchers from all RCs and the MM activity to ensure that the outcomes are relevant to and benefit science across the SFA. There are several science motivations/goals for the FY22 spatial study. For example, it will provide a field-based evaluation of RC-1 basin-scale predictions of hyporheic zone aerobic respiration rates. This will be achieved through sensor deployments, spot measurements of water column respiration, lab measurements of sediment respiration (in collaboration with RC-4's ICON-ModEx effort), and in situ deployment of organic matter decomposition proxies (i.e., cotton strips). The field evaluation of the RC-1 predictions is key to the SFA's ModEx approach. In FY23, deviations from predicted rates will be used to guide modifications to RC1 basin-scale models. The spatial study will cover 48 sites in the YRB that span a broad range of predicted respiration rates as well as stream orders, biomes, climate regimes, and land use/cover influences. This large environmental breadth is key to strong evaluation of model predictions. In addition, the spatial study will provide water chemistry data to further test RC-1 models and provide a large data set in FY22 to the ICON-ModEx effort. Those data will be used in FY22 to update the artificial intelligence (AI) models that predict variation in sediment respiration. The resulting AI predictions will be heavily influenced by patterns in the YRB, thereby benefiting RC-1's efforts to incorporate spatiotemporal variation in sediment respiration rate parameters across the YRB. An EMSL proposal was submitted in FY22 to support molecular analyses of water and sediment samples from the spatial study to further enable mechanistic understanding of drivers of respiration and evaluation of spatiotemporal structure of organic matter chemistry and microbial communities. The spatial study is further connected to RC-3 through inclusion of field sites within and outside of recent wildfire burn perimeters. The selection of those sites has been done in close coordination with RC-3 to ensure relevance to both RC-2 and RC-3.

Science outcomes: RC-2 has generated a number of science outcomes in FY22 that span completion of previous efforts, informal collaboration with researchers outside the SFA, and emerging analyses from FY21 components of the temporal and spatial studies. For example, Kaufman et al. (2022) used a novel dissolved oxygen sensor (from OptiO2) with an automated system sampling system to study 4-dimensional dynamics in the hyporheic zone. Through integrated hydrobiogeochemical measurements they found biogeochemical hot moments tied to hydrologically driven threshold-like shifts in hydrobiogeochemical regimes. In another study, Johnson et al. (2022) used riverbed temperature and 4-dimensional geophysics to reveal the heterogeneity in horizontal and vertical groundwater-surface water exchange flows. To do so they resolved a technical challenge imposed by confounding effects of a moving river-surface boundary on raw resistivity data, thereby enabling deeper characterization of groundwater-surface water mixing, which is a key process impacting river corridor biogeochemistry. On the more conceptual side, Little et al. (2022) proposed the integration of information theory into meta-ecosystem ecology as a complement to traditional foci on material and energy flows among and through ecosystems. They proposed a specific, testable hypothesis relating the information content of organic matter to stream order in the context of the River Continuum Concept (RCC). Data from the temporal and spatial studies in FY21 are being used to test this hypothesis, and more broadly understand how and why organic matter chemistry varies across streams at the basin-scale. More specifically, FTICR-MS data from both the temporal and spatial studies have revealed patterns that contrast with the RCC whereby biochemical and functional trait diversity increase strongly with upstream catchment area. These patterns indicate strong influences of large-scale natural (e.g., climate, vegetation) and human-associated (e.g., urban, agriculture) gradients in land use/cover over the biochemical processes associated with organic matter processing. In addition, we leveraged RC-2's previous developments in meta-metabolome ecology (Danczak et al. 2021) to reveal that there are unique deterministic processes that drive organic matter chemistry in mid-order streams, relative to lower or higher order streams. These organic matter analyses comprise two RC-2 led publications that will be submitted in late FY22 or early FY23. Additional analyses of FY21 data, including those from time-series auto-chambers, have revealed that water column respiration rates are very low relative to whole stream respiration. This indicates that in the YRB most respiration in the stream channel is from the hyporheic zone. This is being compared to CONUS-wide estimates of stream metabolism to put the YRB in a broader context, and associated analyses are being collated into an additional RC-2 led manuscript with a likely submission date in early FY23. As one additional example, previously machine learning-based analyses from RC-1 found that riverbed sediment texture is a dominant driver of variation in hyporheic zone respiration rates. To improve estimates of sediment texture, and thus improve predictions of the dominant respiration contributor, RC-2 and MM are collaborating on a study to use field photos to estimate sediment texture. Early results are promising and if shown to work, this approach will be used to crowdsource sediment texture data from across the YRB, the CONUS, and globally via collaboration with WHONDRS (i.e., RC-4).

Data publication: In addition to the science outcomes, RC-2 had a significant effort in putting together four data packages using ESS-DIVE reporting formats. These data packages include data from sensors and physical samples across the temporal and FY21 spatial studies. These data were delivered to RC-1 (and the rest of the SFA) to facilitate basin-scale model development. They are in the process of being published on ESS-DIVE as publicly open/available data packages. Our team has become proficient in the building/compiling of data packages for ESS-DIVE but have nonetheless found that putting these packages together is a very significant effort requiring large amounts of labor across numerous team members. To help with this challenge, we have automated (i.e., via computer scripts) many of the processes of building and filling ESS-DIVE reporting formats.

Plans for FY23

In FY23, RC-2 will focus on three main thrusts. One thrust will focus on analysis of FY21 and FY22 data (and completion of associated manuscripts, along with publishing FY22 data on ESS-DIVE), with a particular focus on the FY22 spatial study. This will be done in collaboration with RC-1 with the objective of helping to guide modifications to RC-1 basin-scale models. The second thrust will be continued monitoring of hydrobiogeochemistry in the YRB. This will be done primarily via continuation of the temporal study and further development and use of auto-chambers for time series of hyporheic zone respiration. The third thrust will focus on collaboration with MM and RC-3 in terms of using mechanistic models to generate refined hypotheses tied to processes governing respiration and nitrogen cycling in hyporheic zone sediments. In turn, field sampling of sediments will be paired with manipulative lab experiments to test the model-refined hypotheses. This is a central tenet of our ModEx approach. That is, use models to generate hypotheses that we then test using field and/or laboratory data/experiments. RC-3 will engage with this effort to bring in the influences of pyrogenic materials, while RC-2 will focus on the impacts of variation in carbon and nitrogen concentrations and organic matter composition. MM will contribute to the modeling needed to refine our hypotheses and in the design of the associated experiments.

Publication Highlight: Dissolved oxygen sensor in an automated hyporheic sampling system reveals biogeochemical dynamics - Many river corridor systems frequently experience rapid variations in river stage height, hydraulic head gradients, and residence times. The integrated hydrology and biogeochemistry of such systems is challenging to study, particularly in their associated hyporheic zones. We developed an automated system to facilitate 4-dimensional study of dynamic hyporheic zones. It is based on combining real-time in situ and ex-situ measurements from sensor/sampling locations distributed in 3-dimensions. In collaboration with OptiO2 (funded via the SBIR program), we integrated a novel dissolved oxygen (DO) sensor into the system. We measured several biogeochemical and hydrologic parameters at three subsurface depths. During the study, episodes of significant DO variations (+/- 4 mg/l) were observed, with minor variation in other parameters (e.g., < +/- 0.15 mg/l NO_3). DO concentrations were related to hydraulic head gradients, showing both hysteretic and non-hysteretic relationships with abrupt transitions between the two types of relationships (Figure 4). These dynamics indicate biogeochemical hot moments that are driven by hydraulic gradients and that are associated with threshold-like shifts in the hydrobiogeochemical regimes. The study also demonstrated the importance of measuring multiple parameters in parallel, though DO was key for identifying/detecting regime shifts.

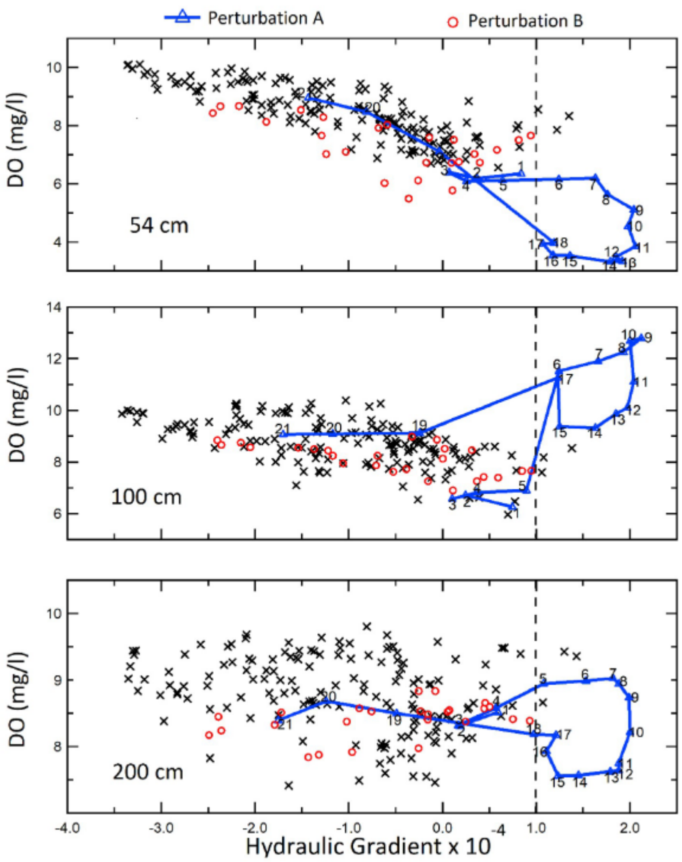

Figure 4 Dissolved oxygen (DO) as a function of hydrologic gradient. Past a given gradient the hydrobiogeochemical regime fundamentally shifts and a biogeochemical hot moment emerges across all three depths surveyed (depth into the hyporheic zone is indicated on each panel).

Reference: Kaufman MH, Ghosh RN, Grate J, Shooltz DD, Freeman MJ, Ball TM, et al. (2022) Dissolved oxygen sensor in an automated hyporheic sampling system reveals biogeochemical dynamics. *PLOS Water* 1(4): e0000014. doi: 10.1371/journal.pwat.0000014.

Research Campaign 3 (RC-3): Watershed Disturbances

Overall Objectives: *The Watershed Disturbances Campaign aims to reveal the mechanisms by which wildfires impact biogeochemical cycling in river corridors from reaction to basin scale.*

- Identify impacts of burn severity: Identify the impacts of burn severity on relationships between pyrogenic material (e.g., PyOM and inorganic nutrients) and river corridor biogeochemistry, with an emphasis on lab-based activities based on BER guidance for changes in RC-3 scope.
- Derive PyOM indicators: Reveal biogeochemical indicators of PyOM derived from different burn severities that can be used for multiscale characterization of PyOM distributions.
- Understand temporal trajectories: Advance the understanding of temporal trajectories of biogeochemical impacts of wildfires within river corridors and their relationship to precipitation.
- Develop PyOM reaction networks: Incorporate the processing of pyrogenic material into reaction network models.
- Relate pyrogenic impacts to watershed features: Lay a foundation for understanding dynamic relationships between pyrogenic materials and river corridor biogeochemistry across variation in watershed features (e.g., stream order and discharge, upland soil physical properties, evapotranspiration, slope of surrounding landscape, and burn area).

Key Contributions of this Research Campaign to the SFA: The River Corridor SFA integrates understanding on the controls of spatial and temporal variations in river corridor hydrobiogeochemistry, its responses to disturbances, and representation in numerical models from reaction to basin scales. To robustly predict changes in watershed function in response to wildfire disturbances, and how those changes will affect water quality and ecosystem health, RC-3 is working on developing a mechanistic understanding of governing processes on the impacts of fires on river corridor hydrobiogeochemistry and will work with RC-1 to further improve model predictive capacity in watersheds impacted by fire disturbances, important for ascertaining the impact of fire on ecosystem structure and function.

FY22 Science Plan Milestone: *In accordance with the changes in budget and scope based on BER guidance, the updated FY22 milestone is as follows:* Complete burn severity leaching experiments. Continue to establish the chemical composition of burned substrates and define associated PyOM indicators in the context of burn severity, focusing on characterizations of PyOC, PyOP, and PyON. Collect spatially distributed and time-series field samples for chemical characterization and analysis of PyOM indicators in post-fire landscapes. Collaborate with RC-1 to incorporate wildfire dynamics into predictive models.

Progress Brief for FY22

Our activities in FY22 are focused on establishing the chemical composition of burned substrates in the context of burn severity, as well as establishing understanding of field-scale in-stream responses to fires.

Identify impacts of burn severity: The major portion of our efforts in FY22 for this activity has been examining results from our burn severity laboratory experiments. Briefly, this work is allowing us to develop an understanding of carbon (C), nitrogen (N), and phosphorus (P) chemical species change with changing burn severities in a controlled setting, through manipulation of feedstocks conditions to simulate low, medium, and high severity burns on open-air burn tables. We leached these materials in artificial rainwater to simulate dissolution of materials that may be transported to the river corridor via overland flow. We conducted nine burns, manipulating fuel moisture, flame duration, and vegetation species to simulate 87 unique combustion conditions. The char sample leachates were analyzed for dissolved organic carbon, major nutrients, and chemical and optical properties of DOM. To date, we have found that higher severity burns had lower concentrations of dissolved C and N than lower severity burns, and that shrubland feedstocks were more soluble than conifer feedstocks. Douglas fir and sagebrush treatments were selected for C, N, P characterization. Muffle furnace burns highlighted unique chemistry of these samples compared to their open-air counterparts; the muffle furnace burns produced less alteration to C and N in the solid chars than low severity open-air burns, with leachate concentrations and chemistries most similar to high severity open-air burns. Together, our findings indicate that different severity wildfires may uniquely impact downstream riverine biogeochemical processes across common wildfire fuel types and that traditional muffle furnace burns do not accurately depict the types of materials solubilized to the river corridor from open-air burning conditions. We are currently working up these results into a series of publications, the first of which will be submitted in late FY22.

Derive PyOM indicators: Several user proposals to enhance our examination of C, N, and P PyOM indicators were successfully funded (SSRL, EMSL and CLS) this FY. Preliminary findings from our SSRL and EMSL user proposals demonstrate distinct molecular signatures with different burning conditions and feedstocks for C, N and P species. NMR of the leachates found the greatest proportion of organic (monoester, diester) and polyphosphates (inorganic) P species are leached in low severity burn conditions, while unburned and moderate severity burns released more orthophosphate (inorganic). In addition, the molecular signatures are unique to feedstock species. Douglas fir leachates had organic P species composed of primarily monoesters including sugar phosphates and phytate, whereas Sagebrush leachates have approximately 5% of organic species as diesters (i.e., DNA). We will continue gathering data from several analysis types for this experiment throughout the rest of FY22 and into FY23 (XANES, NMR, XPS, FT-ICR-MS and targeted biomarkers (e.g., BPCAs)).

Understand temporal trajectories: We are focusing on a targeted sampling response to fires and precipitation though our existing collaborations and monitoring of monthly changes in organic matter chemistry are being investigated in a semi-arid sub-watershed of the YRB (Wenas Creek). Efforts are ongoing to continue monitoring impacts within the 2020 Holiday Farm Fire burn perimeter throughout the recovery process, and our preliminary analyses show more direct organic matter linkages with stream hydrology one year after the fire (2021) compared to the first storm event post-fire in 2020. This represents a strong contrast to the disconnect in hydrology and organic matter chemistry observed in this study that focused sampling efforts immediately following the fire (Roebuck et al., In Review –

publication highlight below). In the YRB, we have continued monitoring the Wenas Creek watershed, to assess inter-annual variability in in-stream response to fire. During elevated flow in the Wenas Creek watershed in Spring and early Summer of 2022, we have been sampling several intermittent tributaries draining burn areas of different severities into Wenas Creek, to assess if increased hydrologic connectivity with these portions of the watershed have impacted in-stream biogeochemistry.

Develop PyOM reaction networks: RC-3 has focused on representing fire impacts in the SWAT watershed model this FY. This work resulted from observations of a negligible difference in-stream water chemistry in fire-impacted portions of the watershed compared to non-fire-impacted parts of the watershed from 2020-2021. Using Wenas Creek as a test watershed, we are working with RC-1 to probe the changes from fires in the landscape and SWAT model parameters necessary to trigger an in-stream response in biogeochemical parameters. RC-3 is also partnering with RC-2 in FY22's spatial study to analyze in situ O_2 rates across fire- and non-fire-impacted sites in the spatial study. This will provide information on if fires might impact observed O_2 rates in relationship to the other land use, land cover, and stream order data sets examined in RC-2 and help to inform future planning of biogeochemical rate examinations and modeling in FY23 (see plans below and in RC-2 FY 23 plans). We also submitted a user proposal to the FICUS program to relate PyOM indicators to microbial community functions across CONUS, leveraging unburned sites in the GROWdb as reference sites in collaboration with RC-4. We plan to incorporate this knowledge into predictions of reaction networks and to revise networks accordingly in FY 24.

Relate pyrogenic impacts to watershed features: This FY we have focused on understanding watershed features through two complementary efforts: 1) The Holiday Farm Fire spatiotemporal monitoring, and 2) The FY21 RC-2 Spatial Study. These efforts examine burn impacts within a single burn perimeter (i.e., common watershed features, ecosystem recovery) and across the entire YRB (i.e., distinct watershed features and time since fire). A detailed description of our recent work in the Holiday Farm Fire can be found in the publication highlight below and our data analysis of the FY21 RC-2 Spatial Study samples is underway.

Publication Highlight: Spatiotemporal controls on the delivery of dissolved organic matter to streams following a wildfire - Our team has recently submitted a manuscript that highlights our ongoing efforts to understand the controls on organic matter transport to streams following wildfire activity and implications for river corridor biogeochemistry. In collaboration with our partners at the Eugene Water and Electric Board (Eugene, OR) and Oregon State University, stream water samples were collected continuously during a major storm flushing event from a series of burned catchments within the McKenzie River basin that were all impacted by varying degrees of burn severity during the 2020 Holiday Farm Fire. DOM chemistry was directly related to burn severity spatially. Organic matter dynamics in the severely burned catchments were distinct from the less severely burned catchments, notable by the increased representation of more aromatic and nitrogen-containing signatures (Figure 5). Furthermore, organic matter signatures observed during the storm were unexpectedly disconnected from shifting hydrological regimes, highlighting the spatially explicit controls of burn severity on the composition of organic materials flushed to streams immediately following a fire. These results suggest there is high potential for wildfires to impact river corridor biogeochemistry on short-term timescales and that in the short-term, spatial DOM dynamics overprint temporal ones immediately following fire activity.

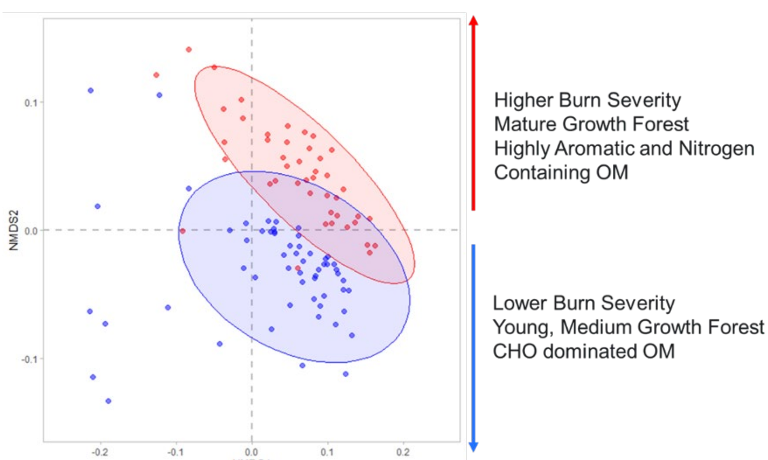

Figure 5 NMDS analysis illustrating the spatial distribution of DOM quality throughout the McKenzie River catchments that were impacted by the Holiday Farm Fire.

Reference: Roebuck Jr., J.A., K.D. Bladon, D. Donahue, E. Graham, S. Grieger, K. Morgenstern, M.J. Norwood, K.A. Wampler, L. Erkert, L. Renteria, R. Danczak, S. Fricke, A. N. Myers-Pigg. "Spatiotemporal controls on the delivery of dissolved organic matter to streams following a wildfire." 2022. In Review at *Geophysical Research Letters*. Pre-print available at doi: 10.1002/essoar.10511361.1

Plans for FY23

In FY23, we will work collaboratively with RC-2 to design and implement coupled fire and non-fire derived biogeochemical reactivity experiments. We will work with MM to develop hypotheses based on model predictions, and design how to test the PyOM influences on C and N coupled dynamics compared to non-PyOM influenced systems in the co-designed lab experiments. We will use this process-based understanding generated herein to define the suite of biogeochemical reactions considered in thermodynamic (Song et al., 2020) and reactive transport models (PFLOTRAN and SWAT-MRMT-R (Fang et al., 2020)) that are impacted by wildfires. We will design and implement a spatiotemporal study in the YRB from the Schneider Spring Fire to further improve model predictive capacity in watersheds impacted by fire disturbances. We will continue our collaborative efforts on monitoring the ecosystem recovery following the Holiday Farm Fire and our burn severity experiment data collection, analysis and publications resulting from this work.

Research Campaign 4 (RC-4): Multi-Basin Studies

Overall Objectives: *The Multi-Basin Studies Campaign aims to provide transferable principles that integrate DOM chemistry, microbial gene expression, biogeochemical function, and disturbance by combining existing global-scale data with WHONDRS-based data generation and numerical modeling distributed across CONUS basins.*

- Expand WHONDRS: Continue to develop WHONDRS as a resource to pursue community-based data analysis, interpretation, and publishing (FY21–24).
- Inform models: Couple DOM chemistry, microbial gene expression, and aerobic respiration in surface and pore water across globally distributed river corridors to inform models in RC-1,2,3 (FY21-23).
- Compare to predictions: Implement ICON-ModEx via crowdsourced sampling designed to test model predictions across CONUS basins and use outcomes to inform further model development (FY22-23).

Key Contributions of this Research Campaign to the SFA: The RCSFA aims to develop predictive capabilities and a fundamental understanding of river corridor hydrobiogeochemistry that apply across basins. This is vital to informing large-scale models that span diverse basins within and beyond CONUS. RC-4 is a key element of this long-term vision by developing transferable knowledge and models. Much of the scientific focus in RC-4 builds from RC-1,2,3 while making more direct use of WHONDRS and expanding the community-based research model that WHONDRS embodies. RC-4 is making use of existing WHONDRS data and growing WHONDRS as a community resource. For example, RC-4 is building the Genome Resolved Open Watersheds database (GROWdb). GROWdb will be an open resource for the community and used by the RCSFA to develop genome-informed mechanistic and reduced order models needed by RC1. In addition, RC-4-generated data are being used by RC3 to contextual PyOM chemistry against a backdrop of natural organic matter (OM). RC-4 is also engaged in numerous crowdsourced sampling campaigns around the globe to generate transferable understanding of factors governing variation in OM chemistry and the biogeochemical impacts of that variation, ultimately to inform the RCSFA's mechanistic and AI models.

FY22 Science Plan Milestone: RC-4 will focus on five primary goals. (1) Generating data and publishing those data on ESS-DIVE from samples collected in FY21. (2) Continue to advance the crowdsourced special collection using WHONDRS data. (3) Implement a crowdsourced sampling campaign based on the integration of ICON principles with a ModEx approach. This ICON-ModEx effort will focus on CONUS riverbed sediment sampling to test and enhance a suite of AI models developed via an SBIR partnership with ParallelWorks. (4) Continue building GROWdb with an emphasis on surface water microbes. (5) Further develop mechanistic and AI models connecting microbes, OM chemistry, biogeochemistry, and hydrology for use in large-scale models.

Progress Brief for FY22

Our activities in FY22 are focused on enhancing transferable knowledge of and predictive capabilities for hyporheic zone sediment respiration, further catalyzing a community of researchers to use and contribute to WHONDRS (meta)data, building a globally-transferable genomics database for river corridors, and formalizing robust (meta)data publication via ESS-DIVE.

ICON-ModEx: The single largest effort for RC-4 in FY22 has been the development and implementation of the ICON-ModEx study of hyporheic zone sediment aerobic respiration. This study is using ICON-based crowdsourced samples (via WHONDRS) to test AI-model predictions of sediment respiration across the CONUS. The generated data not only test the AI-model predictions, they also are being used to update the model's structure and predictions. That 'turning of the ModEx crank' is happening right now. The resulting model/prediction updates will be used to update the CONUS-scale sampling design in real-time. Changes to the sampling design will be acted upon with additional crowdsourced sampling. In addition to crowdsourced sampling, RC-4 is partnering with NEON to pursue time-series sampling across three distinct biomes within the CONUS. This whole research effort has been and continues to be based on ICON principles. For example, the design of the study was openly communicated in video-based, globally open discussions with all that were interested in joining. Feedback from those discussions were used to modify the study plan so that project outcomes (e.g., types of generated data) are high value to those within and beyond the core project team. This ICON-ModEx effort is the largest ModEx effort we are aware of and is changing the paradigm of both ICON-based and ModEx-based science. In essence, this effort is implementing the vision laid out in the 'Open Watershed Science by Design' workshop report. This effort will remain a primary RC-4 effort at least through FY23 and can be scaled up or down as needed, based on resource availability and the technical outcomes of 'turning the ModEx crank' numerous times.

WHONDRS-Local: In FY21 RC-4 had a significant focus on working more closely with collaborators to co-design local-scale sampling campaigns. This is known as 'WHONDRS-Local' and had multiple instances with a focus on environmental contrasts through space and time. For example, samples were taken through time in a small agricultural stream system in the CRB across different hydrologic conditions. In another instance, RC-4 partnered with EXCHANGE (the WHONDRS-like part of COMPASS) and the University of Quebec to study OM chemistry from source to sea along the St. Lawrence River. This effort emphasized numerous environmental gradients and leveraged a long-term research program. These sampling efforts in FY21 generated large numbers of samples and the processing/analysis of these samples has been a major effort in FY22. Many of the data types are now available and efforts are turning to pursuit of publications that will be co-led by the WHONDRS team and the external collaborators that collected the samples. For example, the FTICR-MS data from the St. Lawrence River will be paired with other chemistry data to elucidate coherent shifts in functional properties of OM chemistry moving across water sources and along the fresh-to-saline continuum.

Data generation and publication: RC-4 also continues to generate data from existing and new samples, while also publishing those data on ESS-DIVE. We submitted an EMSL proposal to specifically generate metabolomics data from the 2019 WHONDRS samples. As data move through quality assurance they continue to be added to ESS-DIVE data packages (e.g., sediment mineral composition data from the 2019 campaign were recently added to an existing ESS-DIVE data package).

Completion of prior studies: Multiple RC-4 studies are expected to be completed in FY22. The first major installment of the Genome-Resolved Open Watershed (GROW) database was expected in FY21, but has been delayed due to COVID-19 related backlogs at JGI. It The associated manuscript is expected to be completed in late FY22 or early FY23. This initial paper will focus on surface water microbial communities from global rivers, with a heavy contribution from WHONDRS samples/data. In another manuscript, RC-4 is linking microbial genomes and taxonomy to OM chemistry and inorganic chemistry across global rivers. The associated analyses have revealed strong coordination between microbes and organic and inorganic chemistry. RC-4 is also using CONUS-scale WHONDRS data to test a hypothesis—from the literature—related to OM diversity and respiration rates. The data/patterns are consistent with the hypothesis, though they reveal that the influence of OM diversity is much less than organic carbon concentration.

Open science leadership: RC-4 is continuing to change the paradigm of open science through a globally crowdsourced effort using existing WHONDRS data to study organic chemistry. This effort started in FY21 and continues in FY22, with completion likely in early FY23. Going beyond our previous efforts in crowdsourced publishing, this current effort spans the entire research life cycle from idea generation to data analysis to interpretation and manuscript development. This effort was initially envisioned to result in one crowdsourced manuscript, but we held an initial, open workshop and the high level of interest made it clear that this effort will instead generate an entire special issue of crowdsourced manuscripts all using WHONDRS data. This effort is actively progressing with >100 participants from around the world, and Borton et al. (2022) provides a summary of this effort and the associated vision.

ICON Science: Community outreach is an important part of RC-4, and there have been numerous associated efforts. One significant effort is focused on the continued development of the ICON Science Cooperative and formally establishing its governance (e.g., establishing an advisory board). The Cooperative has partnered, thus far, with EXCHANGE, GROWdb, and WHONDRS, and is in initial stages of developing a partnership with the International Soil Carbon Network. Two major foci of the Cooperative have been developing resources to enable others to use ICON and contributing to new proposals in terms of formal adoption of ICON as the framework through which projects are designed and implemented. The developed resources are being beta-tested by a number of researchers/teams and ICON was used in a recently awarded university-led ESS project. ICON was also used in PNNL's Urban IFL proposal, again as a framework to guide project designed and implementation to achieve mutual benefit and transferable knowledge.

Plans for FY23: In FY23 RC-4 will focus on the following primary goals: (1) Continue the ICON-ModEx effort to generate new mechanistic knowledge and improve predictive models focused on hyporheic zone sediment respiration. (2) Generate data and publishing those data on ESS-DIVE from samples collected in FY22. (3) Complete the crowdsourced special collection using WHONDRS data. (4) Publish the first major GROWdb manuscript summarizing the database and continue building the GROWdb by expanding it to include sediment-associated microbial data, while also facilitating the community to use GROW to generate manuscripts not led by the RCSFA. (5) Further develop mechanistic and AI models connecting microbes, OM chemistry, biogeochemistry, and hydrology for use in large-scale models. (6) Pursue collaborative manuscripts with WHONDRS-Local investigators, with an emphasis on understanding transitions in OM chemistry across environmental contrasts.

Publication Highlight - *It Takes a Village: Using a Crowdsourced Approach to Investigate Organic Matter Composition in Globals Rivers Through the Lens of Ecological Theory* This manuscript serves as an introduction to a crowdsourced collection of research papers that are under development and describes the organization and ideation processes that led to the collection. We held a virtual workshop in April 2021 to engage a community of cross-disciplinary scientists from over 20 countries, 60 institutions, and many career stages with the aim of a multi-perspective, crowdsourced investigation of data from the WHONDRS 2019 sampling campaign. In the workshop, participants generated content for questions, hypotheses, and proposed analyses, resulting in six teams generating research articles in a Frontiers in Water collection. This introductory manuscript brings together summaries of their planned research papers and includes conceptual models representing their hypotheses (Figure 6). This crowdsourced approach to ideation, analysis, and writing lowers barriers for engagement with WHONDRS data, supports new interpersonal connections, and brings together diverse backgrounds to yield innovative ideas. We continue to engage and find new avenues for similar efforts across the RC SFA as we more deeply integrate ICON principles into our work.

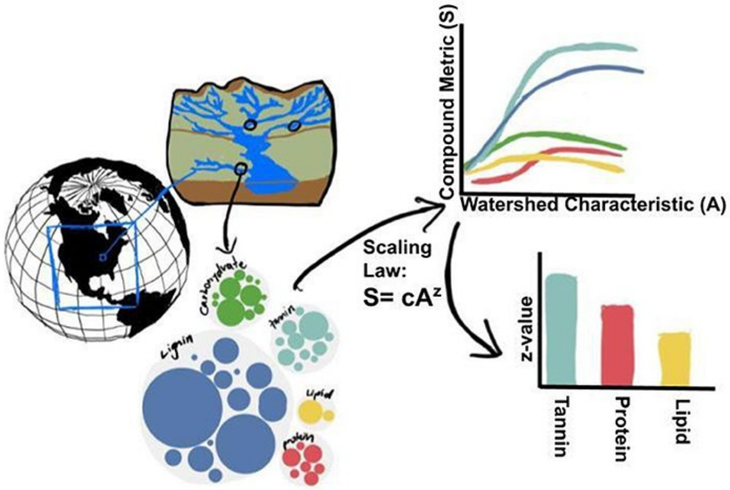

Figure 6 Example of one conceptual model created by the crowdsourced teams. This conceptual model was created from the team working on "Topic 5 – A Unified Conceptual Model of Organic Matter Scaling in River Corridors" and displays their hypothesis linking compound classes associated with decomposition and scaling of watershed characteristics. They are using WHONDRS data to answer the question "Are scaling laws universal such that molecular scaling laws show similar behavior and co-variability to spatial scaling laws?"

Reference: Borton, M.A., S.M. Collins, E.B. Graham, V.A. Garayburu-Caruso, A.E. Goldman, M. de Melo, L. Renteria, J.C. Stegen, and WHONDRS Crowdsourced Consortium. "It Takes a Village: Using a Crowdsourced Approach to Investigate Organic Matter Composition in Global Rivers Through the Lens of Ecological Theory." 2022. *Frontiers in Water*. doi: 10.3389/frwa.2022.870453

Multiscale ModEx:

Overall Objectives: *The MM cross-cutting activity aims to coordinate model–data integration across RCs and scales, assuring optimal use of data and models and open distribution of SFA products.*

- Steward interactive data–model integration (ModEx) across scales and all RCs.
- Implement the Data Management Plan (DMP) and Software Productivity and Sustainability Plan (SW-PSP); provide tools for accessing data and software products.

Progress Brief for FY22

In FY22, the MM cross-cutting activity is focused on 1) incorporation of thermodynamics and redox chemistry into models of OM respiration and nitrogen cycling; 2) application of AI/ML approaches to develop transferable understanding of river corridor hydrobiogeochemistry; 3) implementation of our Data Management and Software Sustainability plans; and 4) development and application of fundamental river hydrodynamics simulations across scales (Figure 7). This activity does not have specific milestones.

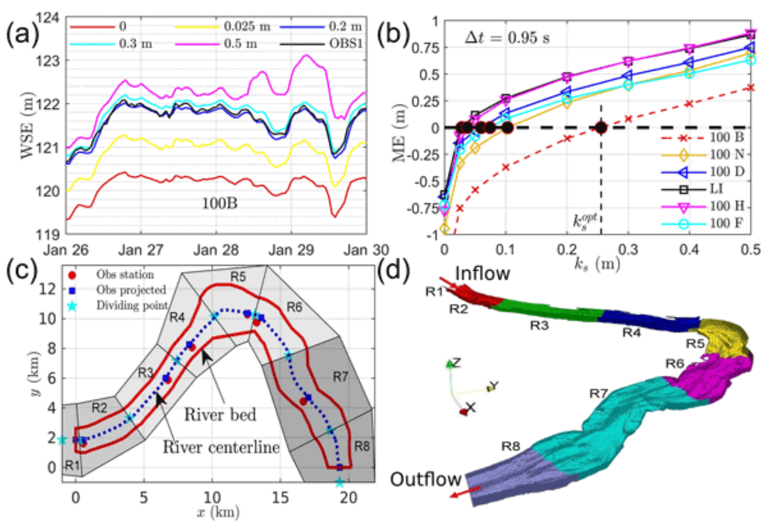

Figure 7 (a) The effect of roughness height on water surface elevation (WSE) at a single location; (b) the mean error between modeled and observed WSE at six locations; (c) the procedure of generating eight roughness regions; and (d) the 3-D view of each region represented in mesh format.

Reference: Chen, Y., J. Bao, Y. Fang, W. A. Perkins, H. Ren, X. Song, Z. Duan, Z. Hou, X. He, and T. D. Scheibe. "Modeling of streamflow in a 30-km long reach spanning 5 years using OpenFOAM 5.x." 2022. *Geoscientific Model Development* 15(7): 2917-2947, doi: 10.5194/gmd-15-2917-2022.

Publication Highlight: High-resolution transient simulation of fully 3-D river hydrodynamics in the Hanford Reach - Developing accurate and efficient modeling techniques for dynamic streamflow at large spatial and temporal scales is essential to evaluating HEFs and their reach-scale impacts. We successfully simulated transient flow over a 5-year time scale and 30-km reach length in the Hanford Reach of the Columbia River using OpenFOAM, an open-source computational fluid dynamics platform (Figure 7). Model results were validated against observations of river stage and velocity and were used to evaluate the relative importance of dynamic and hydrostatic components of pressure at the riverbed. The model provides critical inputs to mechanistic PFLOTRAN simulations of HEFs and biogeochemical reactions and can be used as training data for ML-based surrogate models.

Publication Analysis

78 peer-reviewed journal articles have been published during the current triennial period (2020, 2021, and 2022 to date - see Appendix A for a complete list). Additionally, one journal article and one book chapter have been accepted and 22 manuscripts have been submitted as of the writing of this document. As shown in Figure 8, this is similar to the number of publications in the first two years of the previous period for the last triennial cycle (2017-2019), and is maintaining the same rate of publication in the third year (in contrast to the previous period in which the rate decreased in the third year). It also represents a significant increase over the period 2014-2017. Over the current period, the SFA published most frequently in *Frontiers in Water* (9 papers) and *Water Resources Research* (8 papers). Outside of these two journals, the remaining papers were published in 44 different journals, reflecting the diversity of SFA research and the wide audience reached by our publications. The SFA publishes in high-quality journals: Four publications are in DOE-designated high-impact journals (one in *Nature*, one in *Nature Biotechnology*, and two in *Nature Communications*), 42% of the publications are in ISI-designated top ten journals in their respective fields, more than three-quarters (82%) are in first quartile journals, and nearly all (98%) 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 6.89, a 21% increase from the value of 5.71 reported in 2021.

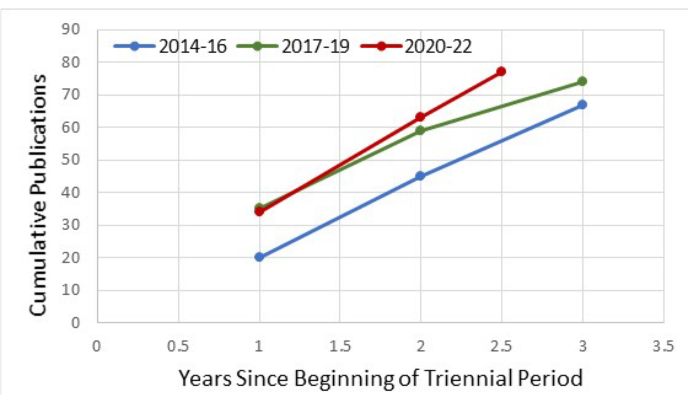

Figure 8. Comparison of number of publications to date in the current performance period (2020-2022) with number of publications in the two previous triennial periods (2014-16 and 2017-19). Note that the point for 2022 is plotted at the elapsed time corresponding to June 30 when this report was submitted and does not include manuscripts that are in press or in review.

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

The Environmental System Science program examines complex ecological and hydro-biogeochemical processes within terrestrial and coastal systems to understand inherent and emergent properties of changes to Earth and environmental systems.[1] The long-term vision of the SFA, closely aligned with ESS objectives, will culminate in transferable understanding of critical hydrologic, biogeochemical, and ecological processes in river corridors, and in the creation of a new broadly applicable simulation capabilities, linked with other watershed hydrobiogeochemical system component models, to provide predictive understanding of watershed function and response to disturbances. In the current performance period (FY21-24), we are expanding our research to study the YRB, which encompasses a broad range of physiographic and hydrobiogeochemical environments. We continue to strengthen our broad

[1] https://ess.science.energy.gov/

collaborations, e.g., through WHONDRS and other efforts, to support generalization of new knowledge, as embodied in numerical models, across the CRB and the CONUS, and integration of those models with major community Earth system model frameworks such as E3SM and the National Water Model.

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

FY22 is the second year of the current performance period for which our research plan was reviewed in 2020. The plan is currently being implemented largely as written, with the exception of modifications made in response to reviewer comments and BER guidance[1]. No near-term major changes in direction or activity plans have been identified at the current time. We conducted a stocktaking meeting in January 2022 to develop more detailed plans and timeline for FY22-24 and make decisions regarding potential expanded geographical scope. Based on that meeting and results to date, we will continue to focus our research in the YRB, with the exception of RC-4 which incorporates the WHONDRS and ICON-MODEX efforts. An emerging scientific theme is the role of non-perennial streams in watershed hydrobiogeochemical cycling. For example, one of our fire-impacted sites in the YRB (Wenas Creek) is normally hydrologically disconnected from the terrestrial landscape due to its arid nature. However, in 2022 we observed significant flow in intermittent tributaries that interacted strongly with the burned regions. Non-perennial streams are one type of variably inundated environment (others include coastal systems, vernal ponds, floodplains, and wetlands). In previous SFA research (Goldman et al., 2017; Song et al., 2021), we have studied the impacts of temporally variable inundation cycles in river parafluvial zones; this research interest is expanding toward other variably inundated watershed subsystems. The SFA led the Variably Inundated Environments Workshop on May 4–5, 2022 with co-leaders Daniel Allen (Penn State Univ.) and Amy Burgin (Univ. of Kansas). The workshop was attended by approximately 40 persons from the research community and we are currently working on a manuscript based on the workshop outcomes.

Collaborative Research Activities

The SFA is dedicated to implementing principles of open, collaborative, integrated team science. We have dramatically increased our collaborative footprint over the past several years through a number of avenues including (1) direct-funded (by subcontract) collaborations with universities, other national laboratories, and other federal agencies (e.g., USGS); (2) collaborative projects funded through SFA FOAs to university partners; (3) collaborative projects funded through the SBIR program; and (4) extensive community-oriented science activities. A detailed list of collaborative projects and activities with co-PI names, institutions, and titles is provided in Appendix B.

Data Management Plan

The River Corridor SFA has a dedicated data management (DM) team funded under the MM activity to support the entire project in implementing our DMP, which adheres to the SC and BER data management requirements. The DM team has established standardized processes (requirements and recommendations) consistent with the DMP that are followed by all RCs. DM team members support individual researchers in creation of data packages associated with publications and/or data collection campaigns and their open publication on the ESS-DIVE repository. All data packages follow the community reporting formats developed by ESS-DIVE with the ESS community.

[1] PNNL SBR SFA Reponses to the Triennial Review Comments, Transmitted to BER October 12, 2020,

APPENDIX A: PROJECT PUBLICATIONS

2022 (as of June 30)

Published:

1. Apte S. V., Oujia T., Matsuda K., Kadoch B., He X. and Schneider K. (2022) Clustering of inertial particles in turbulent flow through a porous unit cell. *Journal of Fluid Mechanics*, **937**, A9; doi: 10.1017/jfm.2022.100.
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8. Johnson T., Thomle J., Stickland C., Goldman A. and Stegen J. (2022) Riverbed temperature and 4D ERT monitoring reveals heterogenous horizontal and vertical groundwater-surface water exchange flows under dynamic stage conditions. *Frontiers in Earth Science*, **10**; doi: 10.3389/feart.2022.910058.
9. Kaufman M. H., Ghosh R., Grate J., Shooltz D., Freeman J., Ball T., Loloee R., McIntire C., Wells J., Strickland C., Vermeul V. R., Rod K. A., Mackley R. D., Lin X., Ren H. and Stegen J. (2022) Dissolved oxygen sensor in an automated hyporheic sampling system reveals biogeochemical dynamics. *PLOS Water* 1(4): e0000014, doi: 10.1371/journal.pwat.0000014.
10. Leonard L. T., Vanzin G. F., Garayburu-Caruso V. A., Lau S. S., Beutler C. A., Newman A. W., Mitch W. A., Stegen J. C., Williams K. H. and Sharp J. O. (2022) Disinfection byproducts formed during drinking water treatment reveal an export control point for dissolved organic matter in a subalpine headwater stream. *Water Research X*, 15, 100144; doi: 10.1016/j.wroa.2022.100144.
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Submitted:

1. Bao Y., Feng Y., Stegen J., Wu M., Chen R., Liu W., Zhang J., Li Z. and Lin X. (2022) Integrating assembly processes, community patterns, and ecosystem function in the context of organic matter degradation. *Nature Ecology & Evolution*, Submitted; 6.13.19.
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16. Son K., Fang Y., Gomez-Velez J. D. and Chen X. (2021) Spatial microbial respiration variations in the hyporheic zones within the Columbia River Basin. *Journal of Geophysical Research. Biogeosciences*, Submitted.
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18. Yang J., Ye M., Chen X., Dai H. and Walker A. (2022) A new total-effect process sensitivity index to identify influential system processes under process model and parametric uncertainty. *Water Resources Research*, Submitted.
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APPENDIX B: DETAILED LISTING OF COLLABORATIVE PROJECTS

Direct-Funded Collaborations – The SFA has directly funded the following external collaborations during FY20-22 to date:

- (2017-Current) Heping Liu, Washington State University – Install, maintain, and process data from eddy flux towers at multiple locations (RC-1).
- (2017-Current) Jesus Gomez-Velez, Vanderbilt University – Develop and apply the NEXSS model and other analytical methods to evaluate HEFs and link to other modeling efforts (RC-1, RC-2, MM).
- (2019-Current) Kelly Wrighton, Colorado State University – Collaborate on microbial community analysis including metagenomics studies for WHONDRS (RC-4).
- (2019-Current) Mark Mastin, US Geological Survey – Install and maintain river water quality monitoring system and incorporate data into USGS water data system.
- (2020-Current) Hyun-Seob Song, University of Nebraska Lincoln – Develop methods for integrating multi-omics data into reactive transport models, and link to other modeling efforts.
- (2021-Current) Bob Hall, University of Montana – Collaborate on design, modeling and interpretation of riverine respiration autochamber data

ESS-Funded University Collaborations – The SFA has collaborated closely with several university-led projects funded by the ESS program during FY20-21:

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

- (FY19-21) 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
- (FY17-20) Michael Gooseff (University of Colorado) Quantifying Distributed Exchanges of Groundwater with River Corridors
- (FY20-22) Matt Ginder-Vogel (University of Wisconsin) Particulate Organic Matter (POM) Transport and Transformation at the Terrestrial-Aquatic Interface

WHONDRS – Collaborative relationships within WHONDRS are too numerous to list.

SBIR-Funded Industrial Collaborations – The SFA works with a number of small businesses to apply and test new field, laboratory and modeling technologies. For example, we are teaming with Parallel Works, Inc. on a SBIR Phase II project "A Platform for Scientific Data Management, Modeling and Analysis with Machine Learning" in support of the ICON-ModEx effort.

Community-level Collaborations:

- Workshop Leadership: SFA team members co-led the Variably Inundated Environments Workshop (VIEW) May 4-5 (described above). Xingyuan Chen chaired the cross-cut session "Knowledge Discovery & Statistical Learning" as part of the 2021 Artificial Intelligence for Earth System Predictability (AI4ESP) workshop series.
- 2022 ESS PI Meeting: Amy Goldman gave an invited plenary lecture: Data Sharing & Open Science: WHONDRS, ICON, & ModEx. Allison Myers-Pigg, Tim Scheibe, and Kevin Bladon co-led (with Michelle Newcomer, LBNL) a breakout session on "Feedbacks between wildfires & ecosystem processes." James Stegen co-led (with Margaret Zimmer, UCSC) a breakout session on "Variable inundation across systems & scales: Towards conceptual & theoretical unification."

- ESS Cyberinfrastructure Working Groups: Co-PI Xingyuan Chen represents the SFA on the Executive Committee and co-leads the Data-Model Integration working group, and other SFA team members participate in working group activities.
- ESS-Dive: The SFA has published numerous public data packages on the ESS-Dive repository in accordance with our DMP.
- KBase and EMSL: SFA collaborator 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-Watersheds: Co-PI Xingyuan Chen is the PNNL lead for the IDEAS-Watersheds collaborative project. Under this project the SFA is co-funding a post-doctoral associate working on development of community cyberinfrastructure.
- ExaSheds: Co-PI Xingyuan Chen is the PNNL lead for the ExaSheds project, which is developing next-generation high-performance watershed modeling capabilities that are integrated with and informed by artificial intelligence methodologies.
- WHONDRS Network: WHONDRS is 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. WHONDRS is coordinated by the SFA, and information on current activities is described above under RC-4. WHONDRS is linked with the GROW[1] network led by Kelly Wrighton (Colo. State Univ.).
- ICON Science Cooperative: James Stegen and Amy Goldman co-founded (with Sujata Emani, USDA-ARS) the Integrated Coordinated Open Networked (ICON) Science Cooperative, and WHONDRS is a partner in the Cooperative with Exchange (COMPASS-FME project) and GROW project led by Kelly Wrighton. The Cooperative is working to enable the broad use of ICON principles (founded in the ESS workshop on Open Watersheds by Design) across science sectors, to dramatically accelerate scientific progress while enhancing equity. For more information, see https://www.pnnl.gov/projects/icon-science.
- Crowdsourced Paper Collection: Kayla Borton, James Stegen, and Amy Goldman are co-editing (with Sarah Collins, Univ. of Wyoming and Michaela Ladeira de Melo, University of Quebec at Montreal) a research topic in *Frontiers in Water* entitled "Crowdsourced Understanding of Global River Organic Matter Composition through the Lens of Ecological Theory." This effort was initiated by a workshop led by the SFA that generated a number of science questions that could be addressed using the WHONDRS OM chemistry dataset. The overview article has been published (Borton et al., 2021) and several contributions from the community are in review or in preparation.
- ICON/FAIR AGU Collection: The SFA organized a special collection hosted by the AGU open access journal *Earth and Space Science*. The collection, entitled "*The Power of Many: Opportunities and Challenges of Integrated, Coordinated, Open, and Networked (ICON) Science to Advance Geosciences,*" comprises commentary articles representing different geoscience disciplines as represented by 19 different AGU sections. In addition to the overview article (Goldman et al., 2022), SFA team members have participated in two other papers to date that are part of the collection (Dwivedi et al., 2022; Hills et al., 2022).
- PyOM Community Review Paper: Allison Myers-Pigg is leading the development of a community review paper on the topic of "*Shaping the future of wildfire science: Top priorities and unanswered questions on the cascading watershed impacts of fires.*" The development of the manuscript is engaging a broad spectrum of researchers using a crowdsourced approach.
- RDPP and RENEW Programs: The SFA is actively participating in new BER programs aimed at increasing participation in BER research programs by underrepresented institutions and populations.

[1] https://jgi.doe.gov/csp-2020-microbial-genomes-across-world-rivers/

- We collaborated with Allison Veach of the University of Texas San Antonio (a minority-serving institution with no recent BER funding) on a proposal to the Research Development Partnership Pilot program (DE-FOA-0002688) entitled “Dissection respiration and carbon flow in intermittent, urban rivers using novel chamber methodologies.”
- We are currently developing preapplications with two MSI partner institutions (Heritage University – a Native American and Hispanic-serving institution in the Yakima River Basin – and UT San Antonio)

- Engagement with Yakima River Basin Stakeholders: We have made significant progress in engagement with a variety of stakeholder institutions in the Yakima River Basin. The SFA regularly participates in meetings of the Yakima River Basin Water Enhancement Project (https://www.usbr.gov/pn/programs/yrbwep/) coordinated by the US Bureau of Reclamation, and of the Yakima River Water Quality and Habitat Coordination Group coordinated by the Benton Conservation District (https://www.bentoncd.org/copy-of-projects). In addition, we are collaborating closely with the agencies to mutually enable field efforts, such as through shared instrumentation and co-design of field efforts. We also hired a PhD intern from Washington State University to work on the spatial study as a complement to his work with the Benton Conservation District on stream metabolism in the YRB. We have received formal permission from the Yakama Nation Tribal Council to perform field work on tribal lands, and we frequently interact with scientists from the Yakama Nation Fisheries including participation by their staff in our field activities. We are in discussions with the Yakama Nation in terms of how they might use data from our field efforts and how they would like to be acknowledged in published data packages and peer-reviewed manuscripts as large portions of SFA data come from their lands. We have made contacts at Heritage University, a Native American and Hispanic-serving institution with campuses in Toppenish WA (on Yakama Nation lands) and Pasco WA (in the Tri-Cities) and are working on joint proposals and student internship possibilities. The SFA further hired a post-doc to develop science communication/outreach materials/strategies. His current focus is developing materials for the data packages from the RC-2 FY21 spatial study to facilitate engagement on the FY22 spatial study, the temporal study, and the SFA’s broader research efforts. These will soon be iterated on with the Yakama Nation to ensure they are culturally sensitive and appropriate for use across a broad range of stakeholders.
- Collaborative science outcomes: RC-4 has generated several science outcomes in FY22 in collaboration with researchers outside the formal SFA structure. For example, Ward et al. (2022) developed an inductive approach to holistic synthesis of river corridor observations using machine learning methods. This revealed unrecognized, strong connections between organic matter chemistry (via FTICR-MS data) and numerous aspects of watershed and river corridor physical, chemical, and biological environments. In another study, Leonard et al. (2022) used synoptic sampling near Crested Butte, CO to identify a biogeochemical hotspot for organic carbon export. Using FTICR-MS and other data types, this fundamental result was extended to reveal controls over disinfection byproduct formation, with relevance to watershed and water quality management. In terms of model development, Rubinstein et al. (2022) developed the ‘Omics to Reactive Transport (ORT) workflow that uses metagenomic and environmental data to describe the effect of microbiological processes in macroscopic reactive transport models. The workflow couples KBase with PFLOTRAN and was demonstrated using microbiological drivers of nitrification and denitrification to predict nitrogen cycling patterns. ORT can be used with spatiotemporal metagenomic datasets—like those being developed in the GROW database—to allow for iterative coupling between KBase and PFLOTRAN. With a stronger focus on physical sample methods, Nelson et al. (2022) studied the impacts of sample treatment on characterization of riverine dissolved organic matter using FTICR-MS. This revealed that the method commonly used by WHONDRS and EMSL are indeed the best single methods for characterizing organic matter unless the focus is on lipid-like compounds, in which additional recommendations were provided. To help catalyze use of WHONDRS data Borton et al. (2022) summarized a crowdsourced collection of research articles all using the same WHONDSR FTICR-MS dataset to study river corridor organic matter chemistry. This represents a fundamentally different

way of doing science in which FAIR (meta)data are provided openly and researchers are brought together to crowdsource manuscripts across a broad range of coordinated topics.

APPENDIX C: REFERENCES CITED

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