Watershed Dynamics and Evolution (WaDE)

ORNL Science Focus Area 2023 Annual Report

Advancing predictive understanding of how dominant processes controlling watershed hydro-biogeochemical function operate under a range of hydrologic regimes and vary along stream networks that drain heterogeneous land covers

Contents

SFA Contact and Sponsor

Contact: Eric Pierce, Oak Ridge National Laboratory, pierceem@ornl.gov

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ESS Environmental System Science

Watersheds are complex systems that provide important ecosystem services. These systems supply freshwater resources for energy production, irrigated agriculture, industry, human consumption, and other ecosystem services. The economic and societal importance of watersheds—and their vulnerability to environmental stresses—is exemplified in the southeastern region of the United States. This region, which includes the Tennessee and South Atlantic–Gulf States water resource regions (WRRs), comprises large areal-extent coastal and inland low-lying areas, elevated plateaus and highlands, numerous high-growth metropolitan areas, and substantial rural expanses. Furthermore, the southeast region is a North American biodiversity hotspot and home to numerous biologically diverse ecosystems.

The Tennessee River Basin in the southeastern United States is the most intensively used freshwater WRR in the contiguous United States, supporting ~4.5 million people with estimated withdrawals of >280,000 gallons per day per square mile. Water resources in the Tennessee River Basin and broader southeastern region are vulnerable to changes in land use and land cover and a range of climate-induced disturbances. Projections indicate that the southeastern United States will experience higher temperatures, more extreme heat events, and an intensifying hydrologic cycle with more frequent and severe storm and drought events over time. The impact of these disturbances is exacerbated by existing regional socioeconomic stressors and inequalities.

To address these changes, the Watershed Dynamics and Evolution (WaDE) Science Focus Area (SFA) at the U.S. Department of Energy's (DOE) Oak Ridge National Laboratory (ORNL) aims to advance predictive understanding of how dominant processes controlling watershed hydro-biogeochemical function operate under a range of hydrologic regimes and vary along stream networks that drain heterogeneous land covers (see Fig. 1, this page).

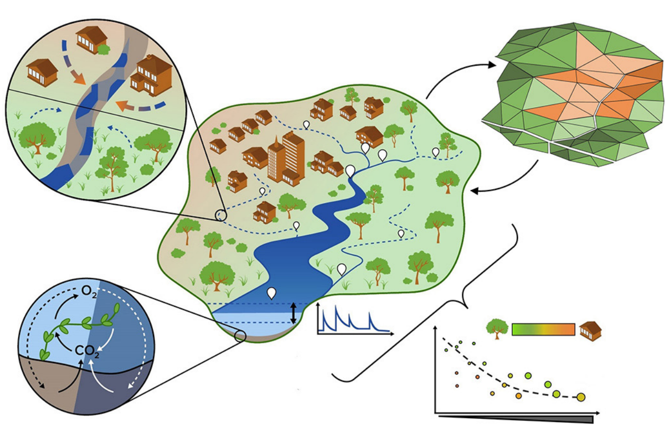


Fig. 1. Research Foci. Conceptualization of 9-year research foci needed to support transferable understanding of watershed hydro-biogeochemical function within and across stream networks that drain heterogeneous land covers: non-perennial dynamics, contributions to stream metabolism, network-scale emergent behaviors, and responses to hydrologic events.

SFA Knowledge Gaps

Process-Based Understanding of Land Cover Effects on Watershed Function. Researchers do not understand if, how, or at what scale land cover influences the generation and export of water and solutes from the landscape to the stream network and how this affects local and emergent hydro-biogeochemical function within the stream network.

Process-Based Understanding of Hillslope-Catchment Interactions. Researchers do not fully understand what controls upland-stream interactions and how these interactions vary under different hydrologic regimes and land covers.

Process-Based Understanding of Integrated Measures of Watershed Function. Researchers have an incomplete understanding of how measures of stream function, such as stream metabolism, integrate complex watershed properties that vary in space and time.

Stream Observational Networks in the United States. Existing observational networks are skewed to higher-order streams and underrepresent low- to mid-order streams.

Watershed Observational Networks in the United States. The watershed science community has largely focused on end-member systems—forested, agricultural, and highly urbanized areas—and researchers currently lack sufficient observations in watersheds with heterogeneous land cover.

Integrated Modeling. Model predictions of watershed function at basin or continental United States scales under changing climate scenarios are uncertain because mechanistic understanding of how key processes depend on land cover and hydrologic regimes is incomplete.

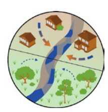
Research Themes

The WaDE SFA is organized around three integrated research themes and a crosscutting modeling activity that together create a multiscale, model-observation-experiment framework to enable hypothesis-driven research addressing the knowledge gaps.

Collectively, this framework will advance a deeper, predictive understanding of:

- Hydro-biogeochemical processes and feedbacks that control solute mobilization and export from headwater catchments with heterogeneous land cover (Theme 1).
- Resultant feedbacks between flow, solute concentrations, and stream function in stream corridors (Theme 2).
- Emergent patterns in stream metabolism at network scales (Theme 3).

This annual report summarizes WaDE accomplishments from December 2022 to June 2023. This time frame represents a portion of the first year following the SFA's triennial peer review in November 2022 and acceptance of the revised plan in January 2023 by the Environmental System Science program within DOE's Biological and Environmental Research program (BER).



Theme 1 *Dynamic Headwaters*

Theme 1 investigates how biogeochemical processes respond to variable saturation in non-perennial channels that connect uplands to the perennial stream network. Non-perennial reaches can make up a significant portion of a stream network. They can flow seasonally because of variation in the water table (intermittent) and/or periodically in response to rain events (ephemeral). The control of these streams on local and downstream biogeochemical processes, such as metabolism, are not well understood. We aim to evaluate the response of non-perennial streams to wetting and drying and assess how these dynamics vary with land cover. Theme 1 combines field-based investigations with laboratory experiments integrated with watershed-scale modeling to advance system-scale understanding of stream metabolism. The overarching research questions in Theme 1 are:

- **Question 1.1:** What are the landscape characteristics that control the frequency and duration of flow in non-perennial streams?

- **Question 1.2:** How do carbon and (micro)nutrient mobilization and chemistry vary in response to changes in sediment saturation across different flow regimes?
- **Question 1.3:** How does variable saturation affect microbiological activity and associated nutrient acquisition and transformation?

FY22–FY23 Accomplishments

Over the past 12 months, Theme 1 completed work performed under the Critical Interfaces SFA and transitioned to the new WaDE SFA. Two published papers describe the role of mercury (Hg) speciation in the formation of methylmercury (MeHg) and mercuric sulfide (HgS) by microorganisms. Two additional papers have been submitted reporting on the light-independent degradation of MeHg by phytoplankton and plants. Moreover, we have completed experiments investigating the interaction of methanobactins with Hg and other transition metals. Methanobactins are metal-chelating peptides used by methanotrophs to acquire copper (Cu) for incorporation into Cu-metalloenzymes that catalyze methane oxidation. Methanobactins are known to form strong complexes with transition metals affecting their biogeochemical transformations and bioavailability. We investigated the interaction of methanobactins with Hg, Cu, and several other transition metals using X-ray absorption spectroscopy, density functional theory (DFT) calculations, and isothermal titration calorimetry. The results show distinct coordination geometries for different transition metals. In addition, we describe a mechanism for reducing Cu(II) to Cu(I) by methanobactins. Overall, our results highlight the interplay between geochemistry and microbial processes on Hg transformations and net MeHg production in the environment.

In the past year, Theme 1 also produced multiple publications investigating the role of manganese (Mn) in regulating carbon dynamics in environmental systems. The consensus of this research is that Mn can promote organic matter degradation through multiple pathways, potentially serving as an important control on carbon (C) stocks in soils. Specifically, Li et al. (2022) reacted synthetic-layer and tunnel-structured Mn oxides with a suite of model organic compounds to evaluate the capacity for Mn oxides to sorb and/or oxidize the organic compounds. We determined that interactions between Mn oxides and organic compounds primarily led to C loss as carbon dioxide (CO_2), although select compounds were predominantly immobilized in the solid phase.

Neupane et al. (2023) evaluated how adding soluble Mn to nitrogen (N)-enriched agricultural soils affected grass litter decomposition. We determined that Mn addition temporarily increased CO_2 release and accelerated conversation of litter C to mineral-associated C in N-fertilized soils. Santos and Herndon (2023) used soil and plant datasets reported by the National Ecological Observatory Network (NEON) to evaluate links between Mn and C across the United States. We found that soil C and N stocks were inversely correlated with soil Mn concentrations, suggesting that Mn drives decreased soil C stocks. Results also indicate that foliar Mn is strongly correlated with foliar lignin, suggesting that Mn is linked with decreased decomposability of litter. The implication of this work is that increased Mn bioavailability and accumulation in foliage under moderately acidic soil conditions support fungal decomposition of lignin-rich litter and contribute to lower soil C stocks. Our knowledge of organo-mineral interactions obtained through this work will inform future investigation into redox biogeochemistry in non-perennial stream networks.

Status of FY23 Milestones

In spring 2023, we started fieldwork with a synoptic sampling campaign in East Fork Poplar Creek (EFPC, see Fig. 2, p. 4) and conducted initial laboratory experiments to evaluate the distribution of organic and inorganic phosphorus compounds with colloidal minerals with changing water chemistry. Deployment of stream temperature, intermittency, and conductivity (STIC) loggers is underway to monitor the presence or absence of surface water along multiple non-perennial streams.

FY24 Plans

Having established a synoptic network, our next objective in FY24 is to evaluate spatial and temporal variability in stream flow and chemistry. Fifty STIC sensors will be co-located with synoptic

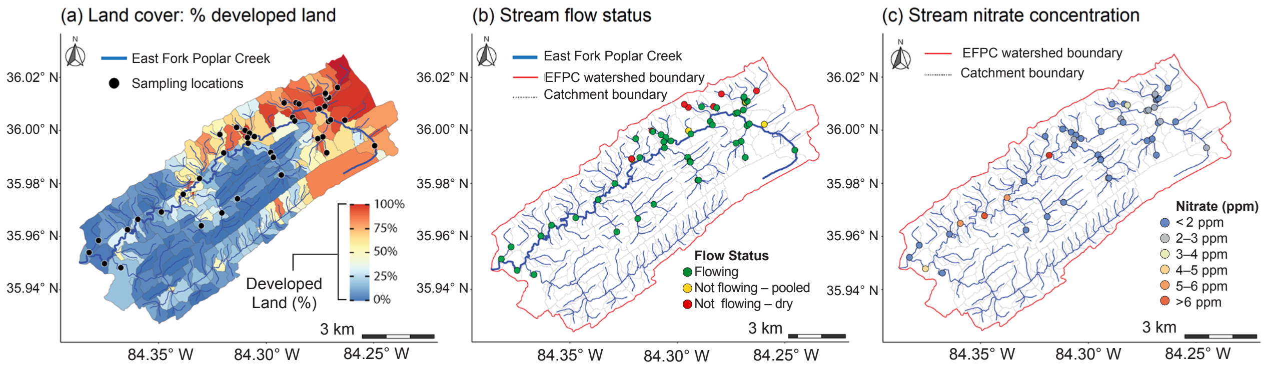


Fig. 2. Initial Site Scouting and Establishment of a Synoptic Survey Network within the East Fork Poplar Creek (EFPC) Stream Network. (a) Initial synoptic sampling locations (black circles) are shown on a map of the EFPC watershed. Subcatchments are color coded by percentage of development, ranging from low (blue) to high (red). (b) Flow status in early April 2023 at each site is marked as no water (red symbols), pooled but non-flowing water (yellow symbols), and flowing (green symbols). (c) Nitrate concentrations at all sites are indicated by color-coded symbols ranging from low (blue) to high (red). Each map shows National Hydrography Dataset (NHD) lines as thin blue lines, EFPC as a thicker blue line, and the watershed boundary as a red line.

sampling sites and used to monitor the occurrence and conductivity of water in the stream channels at high temporal resolution (~15-minute time steps). These data will be integrated with modeling efforts and used to evaluate the expansion and contraction of the stream network and its response to precipitation events across catchments spanning a gradient of land cover (urban to forested). Stream water, when present, will be collected from synoptic sites at least bimonthly and analyzed for nutrients (NO_3^-, NH_4^+, PO_4^{3-}), anions (Cl^-, SO_4^{2-}), major cations (Na^+, K^+, Ca^{2+}, Mg^{2+}), dissolved inorganic and organic C, and a broad suite of trace elements. We will also target these sites for synoptic sampling of microbial communities to evaluate heterogeneity across the stream network.

A second major objective of FY24 is to establish an intensive field site focused on a single non-perennial tributary selected from our synoptic network. We will select a catchment based on catchment characteristics (e.g., land cover), initial evaluations of stream flow and chemistry, and access. Here, we will conduct more intensive measurements targeting understanding of how land cover and underlying geology translate to patterns of stream flow and chemistry from the non-perennial headwaters to the perennial portion of the tributary. For example, we will install water-level loggers, soil-moisture sensors, and redox sensors to evaluate how redox patterns develop in response to flow conditions. We will also analyze the chemical and microbial compositions of surface and subsurface water and riparian soils under different moisture conditions to investigate how stream biogeochemistry responds to wetting and drying.

We will continue laboratory investigations of organo-mineral interactions within the context of colloid aggregation dynamics. Colloids form at redox interfaces in streams and are sensitive to dispersal and aggregation with changes in solution chemistry. These dynamics are poorly understood, though, along with the influence on sorption and reactivity toward organic matter. To investigate coupled physical and chemical dynamics associated with organo-mineral-colloid interactions, we will apply dynamic light-scattering and neutron-scattering techniques in our investigations.

Manuscripts

Published or In Press

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Theme 2
Stream Corridor Processes

Theme 2 studies stream corridor processes at the reach scale using a combination of field experiments, laboratory mesocosm studies, long-term observations, and modeling. Our work is motivated by the knowledge that mid-order streams are reactive conveyors that receive, process, and transport carbon, nutrients, and other solutes from upstream and the surrounding uplands. Although these mid-order streams are a vital link between low-order headwaters and larger rivers, they are noticeably under-represented in the research literature, and thus a quantitative understanding of their roles in watershed function is lacking. The overarching research questions in Theme 2 are:

- **Question 2.1:** How are the relative contributions of water-column versus benthic gross primary production (GPP) and ecosystem respiration (ER) to net ecosystem production (i.e., the balance of GPP and ER) affected by gradients in sediment pollution and nutrient limitation associated with different land covers?

- **Question 2.2:** How do organic matter inputs and burial alter aerobic and anaerobic metabolism in the stream benthos?

- **Question 2.3:** How do transient, high-flow events affect stream metabolism and associated measures of stream function such as C and nutrient spiraling length and uptake velocity? How do these biogeochemical processes vary along gradients of land cover?

FY22–FY23 Accomplishments

During FY22 and early into FY23, Theme 2 completed work performed under the Critical Interfaces SFA and transitioned to the new WaDE SFA. Several manuscripts were published or submitted detailing our research on Hg hydro-biogeochemistry (listed below). Importantly, several of these papers provide a solid foundation for our transition to the WaDE SFA (e.g., Ikard 2023; Buser-Young 2023; Brooks 2023). These papers leverage our broader experiments and data collection to interpret watershed processes relevant to all streams at local and continental scales.

FY24 Plans

Our highest-priority plans for FY23 were enabling objectives upon which our future FY24 efforts depend. These include:

- **Selecting sites for long-term observation records —** All three sites have been identified, and each coincides with dominant land-cover categories within our first watershed (e.g., industrial/urban, suburban, and forested).

- **Installing monitoring equipment —** Two of the three sites have been instrumented with monitoring equipment. Equipment availability for the third site has been impacted by lingering supply-chain issues.

We have initiated the regular water sampling, which supports development of concentration-discharge curves as a function of dominant land cover. Additionally, we have started testing equipment and refining experimental procedures that will be used in the light-dark bottle incubation tests.

Manuscripts

Published or In Press

Brooks, S. C., A. L. Riscassi, C. L. Miller, K. A. Lowe, X. Yin, and T. L. Mehlhorn. 2022. “Diel mercury xconcentration variations in a mercury-impacted stream,” *Environmental Science: Processes & Impacts* **24**, 1195–1211. DOI:10.1039/d2em00142j.

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Johs, A., L. Gonez-Rodriguez, S. C. Brooks, and M. A. Mayes. In review. “Factors controlling the mobilization of mercury from contaminated creekbank soils,” *Journal of Environmental Quality*.

Horita, J., D. B. Watson, S. Toyoda, S. C. Brooks, O. Warr, B. Sherwood Lollar, M. E. Conrad, and N. Yoshida. In revision. “Coupled hydrogeochemical-microbial processes at an acid, radionuclide-contaminated site at the US DOE Oak Ridge Reservation, Tennessee: Implications for bioremediation and life under extreme conditions,” *Geochimica et Cosmochimica Acta.*

Data Products Released

Brooks, S. C., and K. A. Lowe. In preparation. [Data Set] East Fork Poplar Creek Discharge at Kilometer 5.4 Water Year 2021. ORNL Mercury Science Focus Area (SFA) Data Collection, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, USA.

Brooks, S. C., and K. A. Lowe. In preparation. [Data Set] East Fork Poplar Creek Sonde Data at Kilometer 5.4 Water Year 2021. ORNL Mercury Science Focus Area (SFA) Data Collection, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, USA.

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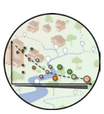

Theme 3 *Network Function*

Theme 3 is investigating the relative drivers and emergent patterns in stream function within and across mid-order stream networks and their response to network position, land cover, and changes in network connectivity resulting from seasonal and event-based flow dynamics. We are utilizing whole-stream metabolism (e.g., gross primary production, ecosystem respiration, and net ecosystem production) as an integrated metric of stream function, estimated using both dissolved oxygen (DO) and CO_2. We are using a range of solutes with differing integration lengths; solutes with short integration lengths (including O_2 and CO_2) will reflect more localized behavior than those with long integration lengths. We are also utilizing synchrony as a framework for evaluating spatiotemporal patterns in stream metabolism in relationship to potential drivers. Theme 3’s research questions are:

- **Question 3.1:** When and where do metabolic regimes synchronize along a stream network, or why do they diverge?
- **Question 3.2:** How do variable inputs of flow and solutes from non-perennial tributaries influence rates of stream metabolism in the downstream mainstem, and how does this effect scale with the length of the flowing network?

FY22–FY23 Accomplishments

Identifying Study Watersheds

In collaboration with the other Themes and Modeling Crosscut, Theme 3 led the selection of the three representative study watersheds that WaDE will focus on over the next 10 years. The project will use these sites to systematically translate, apply, and refine the process understanding and modeling capabilities gained from one watershed to increasingly disparate systems.

To guide the selection of the three watersheds, Theme 3 conducted an analysis to determine representative clusters of mid-order watersheds within the Tennessee River Basin (TRB) based on key characteristics known to influence watershed function. We used the National Watershed Boundary Dataset’s HUC-12 designation as a spatial template to identify 524 headwater HUC-12s within the TRB. We then identified 19 variables from the U.S. Environmental Protection Agency’s StreamCat dataset that best capture key characteristics relating to watershed geography, hydrology, land cover, geology, soils, and ecology. The team then used a k-means clustering algorithm to group watersheds based on their similarity as a function of the 19 variables. We determined that the optimal number of clusters that balances complexity and variability is three based on the elbow method. Lithology, elevation, temperature, and soil clay content showed the most difference among clusters and thus were most important for differentiating watersheds. Repeating this approach with an expanded set of 72 variables did not change the clustering results.

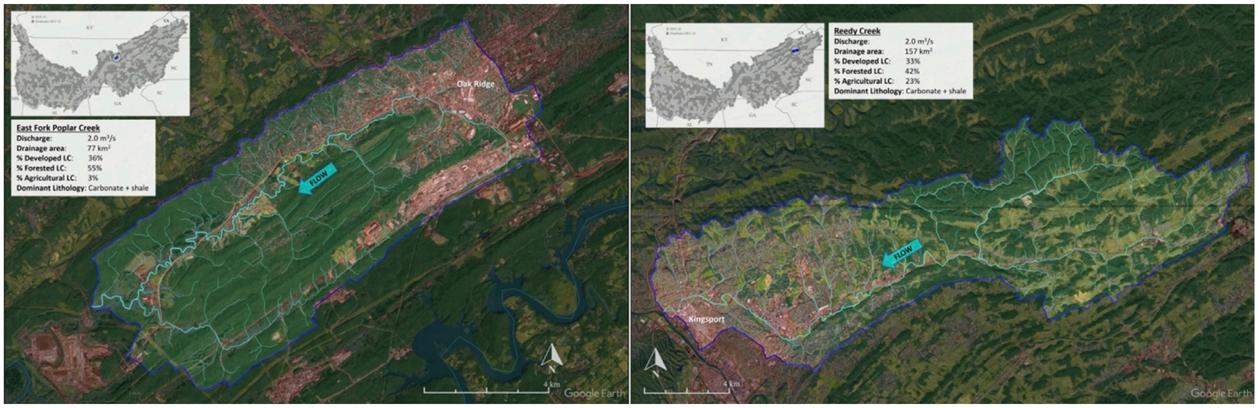

Fig. 3. WaDE's Study Watersheds. Satellite images of the two selected study watersheds, East Fork Poplar Creek (left) and Reedy Creek (right). The land cover color overlay illustrates the opposing gradients of developed cover (pink) to forest (dark green) and agriculture (yellow-green). Inset tables summarize key characteristics of both watersheds.

From these 524 headwater watersheds we down-selected candidate study watersheds based on three land cover–based criteria: (1) <5% open water + wetlands; (2) 20% to 60% development, including >1% high-density development; and (3) forest cover > agricultural cover. We selected two watersheds from within a single cluster (i.e., they share key characteristics known to influence watershed function). Notably, the two watersheds have opposing gradients in land cover: The East Fork Poplar Creek watershed (Tenn.) transitions from urbanized to forest with downstream distance, and the Reedy Creek watershed (Tenn./Va.) does the reverse (see Fig. 3, this page). The third study watershed, still to be determined, will be selected from a second cluster.

Synoptic Evaluation of Regional Watershed Response

The three representative clusters identified in the watershed selection process represent the hypothesis that broad patterns in watershed hydro-biogeochemical response can be predicted by key high-level state and forcing variables. However, we know that local conditions and drivers may outweigh the effects of these high-level variables under certain conditions (e.g., during low flow periods). To test this hypothesis, Theme 3 instrumented the outlet of 25 HUC-12 watersheds spanning the three clusters with DO and conductivity-temperature-depth sensors in March 2023. These instruments will operate for approximately 9 months, spanning leaf-on to leaf-drop. Among other objectives, this dataset will allow us to (1) assess the relative responses of flow, temperature, conductivity, and oxygen to event- and seasonal-scale drivers; (2) evaluate the significance of high-level variables (especially land cover); (3) determine land-cover metrics that best explain observed system differences; and (4) evaluate synchrony in response to leaf-on and leaf-drop. This study is complementary to network synchrony involving the evaluation of spatio-temporal controls on network-scale synchrony/asynchrony in stream metabolism.

Third-Order, High-Frequency DO-CO_2 Sensor Network

Establishment of a "core" sensor network in our first study watershed, East Fork Poplar Creek, is central to both network synchrony and connectivity. To date, Theme 3 has identified and instrumented 14 sites within the perennial stream network that bracket major tributary confluences and land-cover changes. Three of these are Theme 2's long-term observational sites. To support the study of network synchrony, we have initiated monthly water-chemistry sampling campaigns at these sites, often coinciding with Theme 1's sampling campaigns, and monthly deployments of cotton strips to evaluate organic matter decomposition.

FY24 Plans

FY24 work will focus on network synchrony. The core sensor network at East Fork Poplar Creek will be expanded to include conductivity-temperature-depth and dissolved CO_2 sensors at the sites not currently instrumented for these parameters. The monthly sampling campaigns will continue and be augmented by event-based campaigns. We also plan to conduct solute tracer tests at key network nodes to evaluate coupled aerobic respiration and solute transport. We will begin planning for a skeleton sensor network at our second study watershed, Reedy Creek.

The bulk of network connectivity will wait on Theme 1's selection of non-perennial study sites and installation of the wet-dry sensor network. In the next year, Theme 3 will expand the synoptic campaigns to include more non-perennial sites, in collaboration with Theme 1. We also plan to conduct a trial and baseline assessment of nutrient limitation (via nutrient-diffusing substrates) at the core sensor sites. Installation of the expanded non-perennial (non-core) sensor network will occur after the regional watershed sensors are returned in fall 2023.

Manuscripts

Published or In Press

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Theme 4 *Modeling Crosscut*

FY22-FY23 Accomplishments

The Modeling Crosscut is developing a virtual watershed modeling capability to support hypothesis-driven modeling for each theme. The approach is to use the DOE-developed watershed modeling framework with the Advanced Terrestrial Simulator (ATS; Coon et al. 2019) for integrated surface/subsurface hydrology and solute transport coupled through the Alquimia interface (Molins et al. 2022) to PFLOTRAN (Hammond et al. 2014) for biogeochemical reactions. A novel aspect of this work is the use of ATS's multiscale capability to represent the effects of small-scale hyporheic-zone biogeochemical reactions at the appropriate scale using hyporheic age-based subgrid models. The multiscale stream corridor model was developed previously (Jan et al. 2021) as a joint effort between the Critical Interfaces SFA and the IDEAS-Watersheds project and was extended and tested in FY23 (Le et al. 2023). This model avoids *ad hoc* upscaling and explicitly accounts for rate-limiting mass transfer between the flowing channel and biogeochemically active transient storage zones.

Continuing work from the Critical Interfaces SFA, numerical experiments were undertaken to test the feasibility of using photosensitive tracers in day and night injections to separate surface storage and hyporheic-zone storage in streams. Those experiments used ATS's multiscale stream corridor model configured with two subgrid models, one for surface storage and one for hyporheic-zone storage. Results (Rathore et al. 2023) show this is a viable strategy for delineating hyporheic and surface transient storage, provided the tracer has sufficient photoreactivity in the conditions of the test. Moreover, the results show that attempting to interpret tracer tests with an overly simplified model structure (i.e., a single transient storage zone) can result in significant biases in the estimated parameter. More generally, these results show the value of pre-modeling and data-worth analyses in designing time-consuming and expensive field tracer tests and subsequent analysis.

Significant progress was made toward the high-resolution thermal hydrology models of East Fork Poplar Creek. In collaboration with the ExaSheds project, the Modeling Crosscut team re-implemented the streamlight model capabilities (Savoy et al. 2021) in the Watershed Workflow (Coon and Shuai 2022) toolkit, which builds input for spatially resolved ATS simulations. The new capabilities in Watershed Workflow estimate photon flux density incident on the stream channel, considering stream shading by nearby vegetation. Photon flux density is needed both for stream gross primary production estimates and for surface energy balance, which is required for stream temperature simulations. In addition, a high-resolution hydrology model for East Fork Poplar Creek was implemented (see Fig. 4, this page), and the modeling team is in the process of extending that model to include stream temperature.

The Modeling Crosscut team also made significant progress on stream metabolism models. As a reference case, the three-parameter class (Odum 1956) of single-station metabolism models was implemented in the ATS-PFLOTRAN system. Although the reaction model itself is standard, our implementation is unique in that it is made spatially explicit at watershed scales by relying on ATS's solute transport capabilities. We also extended the reaction model to move ecosystem respiration into the hyporheic zone using ATS's stream corridor model to represent rate-limited mass transfer between the stream channel and hyporheic zone, a more realistic representation. The separation of

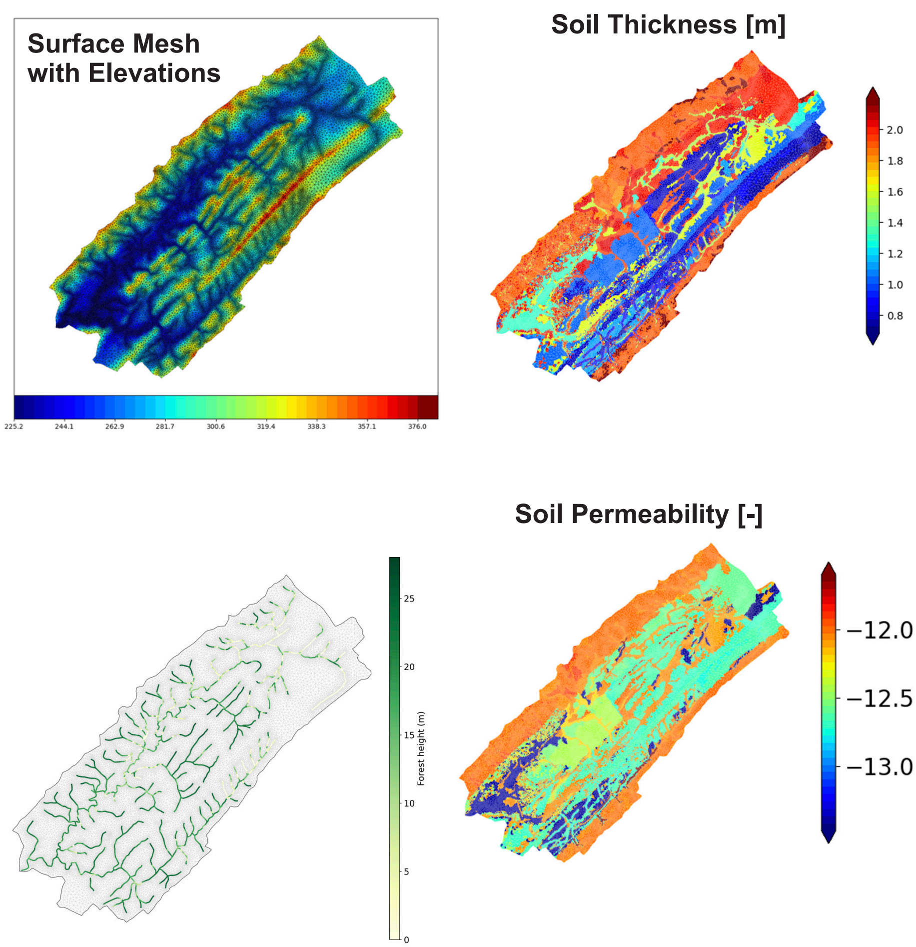


Fig. 4. East Fork Poplar Creek (EFPC) High-Resolution Hydrology Modeling. Clockwise from upper left: computational mesh for an Advanced Terrestrial Simulator (ATS) model of EFPC, soil thickness, soil permeability, and forest height adjacent to the stream network. Soil property inputs to ATS are normally taken from community data products, but those products have data gaps in lower EFPC, so machine-learning imputation was used to fill those gaps. Forest height is an important input to the stream shading model and is used in streamlight to estimate incident radiation on the stream.

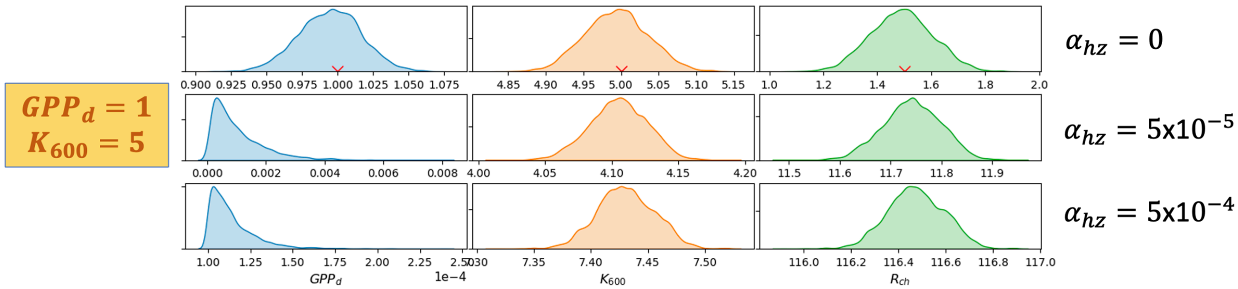


Fig. 5. Results of Numerical Experiments Used to Understand Potential Biases Introduced from Oversimplifying Stream Metabolism Processes in Models. Each row shows distributions of gross primary production (GPP), reaeration rate constant, and ecosystem respiration as estimated from a time-resolved CO_2 signal using the Odum-type three-parameter model and Markov-Chain Monte Carlo. The rows use different assumptions to generate the synthetic truth CO_2 signal with different values for the rate constant for hyporheic exchange. Parameters are recovered with low bias and low uncertainty when there is no hyporheic exchange (top row). However, large biases in the estimated parameters are encountered when mass transfer between the flowing channel and the metabolically active storage zones is ignored.

the mass transfer processes from the reaction model is important for our purposes, as the conventional approach conflates the two and limits transferability.

We are currently using the new capability to understand biases resulting from ignoring mass transfer limitations, as is done in the standard three-parameter model. Specifically, we generated three synthetic truth CO_2 time series using ATS and our multiscale model. The synthetic truth cases have no hyporheic exchange, low hyporheic exchange ($\alpha_{hz} = 5\times10^{-5}$ s^{-1}), and high hyporheic exchange ($\alpha_{hz} = 5\times10^{-4}$ s^{-1}). Here, α_{hz} is the hyporheic exchange rate constant. For each synthetic truth case, we then used the three-parameter model to interpret the signal. Specifically, we used Markov-Chain Monte Carlo (MCMC) to estimate the three model parameters from the CO_2 signal, as in the streamMetabolizer (Appling et al. 2018) package. With no hyporheic zone (α_{hz}=0), the MCMC algorithm correctly estimates the model parameters, as expected. However, in the more realistic case when the synthetic truth case is generated with hyporheic exchange, parameters estimated by the three-parameter model have large biases (see Fig. 5, this page) because the parameter estimation process is attempting to compensate for model structural error by decreasing gross primary production and increasing ecosystem respiration.

FY24 Plans

In FY24, the Modeling Crosscut team will refine our preliminary high-resolution hydrologic model of East Fork Poplar Creek and calibrate it using stream discharge records. We will then extend the ATS-based model to represent stream temperatures, evaluate the new thermal hydrology model using stream temperature records, and prepare a journal article on the results. We will continue to implement stream metabolism models and compare them to dissolved oxygen measurements as they become available.

Manuscripts

Published or In Press

Le, P. V. V., S. S. Rathore, and S. L. Painter. 2023. “A multiscale model for solute transport in stream corridors with unsteady flow,” *Journal of Hydrology* **622**, 129670. DOI:10.1016/j.jhydrol.2023.12967.

Rathore, S. S., A. S. Ward, and S. L. Painter, 2023. In press. “Numerical evaluation of photosensitive tracers as a strategy for separating surface and subsurface transient storage in streams,” *Journal of Hydrology*.

Rathore, S. S., G. E. Schwartz, S. C. Brooks, and S. L. Painter. 2022. “Joint estimation of biogeochemical model parameters from multiple experiments: A Bayesian approach applied to mercury methylation,” *Environmental Modelling & Software* **155**, 105453. DOI:10.1016/j.envsoft.2022.105453.

Selected Research Highlights

In FY 2023, 33 manuscripts were published or submitted by the SFA team. Of these publications, 23 are published or in press. In this section, we highlight three of the 23 published or submitted manuscripts.

Research Highlight

Nitrous Oxide Inhibits Methylmercury and Methane Formation in Arctic Tundra Soils

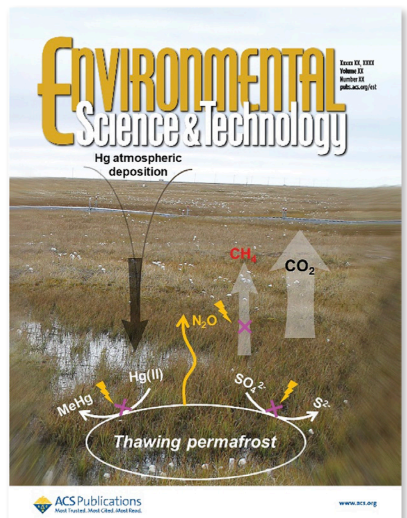
Study highlights the complex interplay of microbial processes that determine how climate change may influence greenhouse gas and toxic methylmercury formation in the Arctic.

The Science

Climate warming causes permafrost thaw predicted to increase methane (CH_4), carbon dioxide (CO_2), and toxic methylmercury (MeHg) formation, as well as nitrous oxide (N_2O), another potent greenhouse gas formed during degradation of nitrogen-containing soil organic matter in the Arctic.

A microcosm incubation study with Arctic tundra soil over 145 days demonstrated that N_2O at concentrations as low as 0.1 mM markedly inhibited microbial MeHg formation, methanogenesis, and sulfate reduction while slightly promoting CO_2 production. Microbial community analyses indicate that N_2O decreased the relative abundances of methanogenic archaea and microbial clades implicated in sulfate reduction and MeHg formation. Following depletion of N_2O, both MeHg formation and sulfate reduction rapidly resumed, whereas CH_4 production remained low, suggesting that N_2O affected susceptible microbial guilds differently.

MeHg formation strongly coincided with sulfate reduction, supporting prior reports linking sulfate-reducing bacteria (SRB) to MeHg formation in the Arctic soil. Our results suggest that microbial production of CH_4, CO_2, and MeHg is more complicated than previously thought. This research demonstrates complex biogeochemical interactions governing CH_4 and MeHg formation and thus lays the foundation for future mechanistic studies for improved predictive understanding of MeHg and greenhouse gas fluxes from thawing permafrost ecosystems.



Permafrost thaw and organic matter degradation could release nitrous oxide, a potent greenhouse gas that in turn inhibits mercury methylation and methanogenesis (methane formation). This research highlights the complex interplay of microbial processes that determine how climate change may influence greenhouse gas and methylmercury formation in the Arctic.

The Impact

We observe that N_2O strongly inhibits MeHg and CH_4 production in Arctic permafrost, which is considered a critical-zone environment for MeHg formation and greenhouse gas (e.g., CH_4, CO_2, N_2O) emissions under climate warming scenarios. The observed inhibitory effects of N_2O have important implications for predicting the formation of neurotoxic MeHg and greenhouse gas emissions in Arctic ecosystems.

Summary

Climate warming causes permafrost thaw and soil organic matter degradation, resulting in the formation and release of CH_4, CO_2, N_2O, and toxic MeHg in the Arctic. We found that N_2O strongly inhibits CH_4 and MeHg formation, suggesting that microbial production of CH_4, CO_2, and MeHg is more complicated than previously thought. The complex interplay of microbial processes ultimately may determine how climate change will influence greenhouse gas formation and mercury transformation in the anoxic Arctic tundra.

Publication

Zhang, L., Y. Yin, Y. Sun, X. Liang, D. E. Graham, E. M. Pierce, F. E. Löffler, and B. Gu. 2023. “Inhibition of methylmercury and methane formation by nitrous oxide in Arctic tundra soil microcosms,” *Environmental Science & Technology* **57**(14), 5655–65. DOI:10.1021/acs.est.2c09457.

Research Highlight

Coupled Electrical Geophysics Methods Identify Where Water Moves Between Groundwater and Surface Water

Noninvasive, nondestructive techniques enable mapping hyporheic exchange in bedrock-lined stream channels.

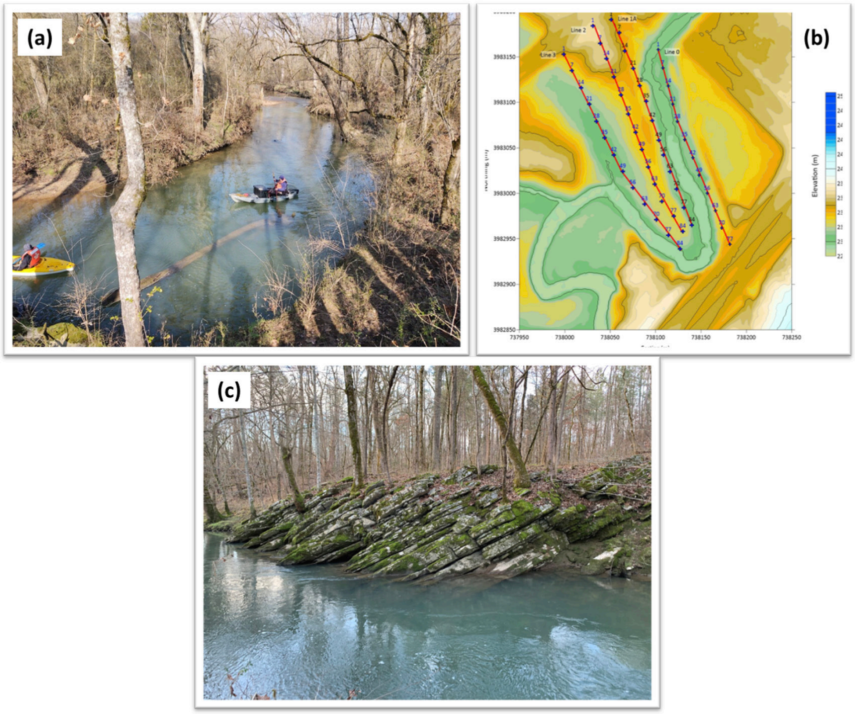
The Science

The hyporheic zone—an area around stream channels where groundwater mixes with surface water—is highly active in the processing and transformation of carbon, nutrients, trace elements, and contaminants. Knowing how and where water moves between the surface and subsurface is essential to understanding the ecosystem services provided by streams and how they respond to changing climate and other anthropogenic activity (e.g., changing land cover).

Previous work to identify the hyporheic zone has focused almost exclusively on streambeds with loose, unconsolidated sediment. New methods are needed to identify these water exchanges in bedrock-lined streams. The WaDE team applied two geoelectric survey methods along a 220-meter reach of the bedrock-lined East Fork Poplar Creek in East Tennessee. Natural electric fields were measured using waterborne self-potential arrays (WaSP), and these identified where water moved between the groundwater and surface water in the stream channel. Artificial electric fields, generated by injecting electrical current into the ground, were used to create images of the electrical properties of subsurface materials using electrical resistivity tomography (ERT). ERT data reveal hidden information about subsurface structure and the hydrogeological setting. Both techniques are noninvasive and nondestructive. Results from the two methods were combined to map and characterize likely locations where water moves between the groundwater and surface water in the stream channel.

The Impact

This study revealed novel insights into groundwater–surface water exchange in bedrock-lined channels by combining two geoelectric survey methods. These noninvasive and nondestructive techniques generate relatively high spatial resolution information over broad spatial scales. The results of this study enable mapping hyporheic exchange in bedrock-lined stream channels and may be able to capture exchange dynamics through time-lapse surveys.



Waterborne self-potential (WaSP) logging (a) and land-based electrical resistivity tomography (ERT) (b) were used together to identify locations where surface water–groundwater exchange was likely occurring along East Fork Poplar Creek in Oak Ridge, Tenn. Water movement between groundwater and surface water aligned with visible bedrock outcrops (c) and hidden underground fractures identified by ERT.

Summary

Knowing where and how water moves between open stream channels and the surrounding subsurface is essential to understanding the role of streams in processing and transporting carbon, nutrients, trace elements, and contaminants. However, current methods to study this water movement are not applicable to bedrock-lined channels. Therefore, the WaDE team applied two geoelectric survey techniques (WaSP and ERT) to map likely locations of groundwater–surface water exchange and interpreted them within their hydrogeological context. Results indicate that these locations aligned with visible bedrock outcrops and, importantly, with hidden underground fractures identified using ERT.

Publication

Ikard, S. J., K. C. Carroll, D. F. Rucker, R. F. Adams, and S. C. Brooks. 2023. “Geoelectric survey of surface-water and groundwater exchange in East Fork Poplar Creek, Oak Ridge, Tennessee,” *Geophysical Research Letters* **50**(8), e2022GL102616. DOI:10.1029/2022GL102616.

Research Highlight

How Much of the Streambed Can We Measure?

Study pioneers new technique to measure commonly unobservable stream flowpaths.

The Science

Solute tracer studies are the most common way to measure the role of the near-stream subsurface, or hyporheic zone, in stream processes. However, such studies are limited in scope and known to be biased toward only the shortest and fastest flowpaths. In contrast, some ecosystem processes of interest only occur along slower or longer flowpaths. Thus, scientists have an incomplete understanding of the hyporheic zone.

In the past, flowpaths beyond a "window of detection" were necessarily overlooked, along with ecosystem processes along these paths. Using a new approach, scientists can quantify what was lost, shattering the former window of detection and including a more complete understanding of hyporheic zones in predictions and forecasts. Ultimately, this study initiates a new approach to stream solute tracers, overcoming a limitation that has plagued the tracer technique for more than 30 years.

The Impact

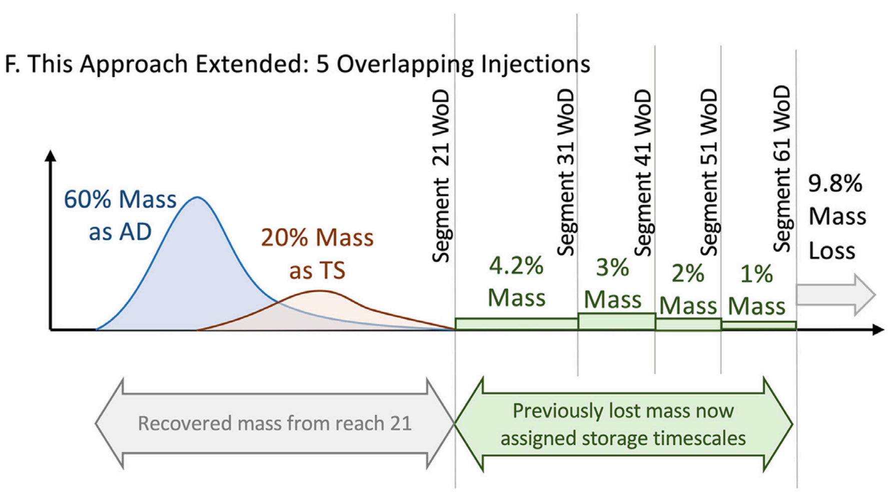
The approach pioneered in this study enables scientists to assess more accurately the timescale of water and solute transport in study reaches. This is a critical variable in predicting the transport, transformation, and fate of nutrients, pollutants, and energy in river corridors.

Summary

Although water and solute transport are known to have timescales spanning orders of magnitude, the full range is seldom observed. Here, a new approach is established to see longer-in-time flowpaths, enabling scientists to systematically probe portions of the system traditionally unstudied.

Publication

Ward, A. S., S. M. Wondzell, M. N. Gooseff, T. Covino, S. Herzog, B. McGlynn, and R. A. Payn. 2023. "Breaking the window of detection: Using multi-scale solute tracer studies to assess mass recovery at the detection limit," *Water Resources Research* **59**, e2022WR032736. DOI:10.1029/2022WR032736.



The techniques established in this study enable assessment of timescales traditionally not included in streambed measurements, enabling more detailed understanding of the transport and fate of nutrients, energy, pollutants, and water in river corridors.

Postgraduate Spotlight

A key goal of the WaDE SFA and ORNL is to develop and train the next generation of scientists and engineers. As part of this year's report, we highlight three of our outstanding postgraduate researchers—Matthew Berens, Kristen Bidas, and Deandre Presswood—who are contributing to WaDE's overall goals and objectives. See website for a complete list of the project's postgraduate alumni (wade.ornl.gov/history/).

Matthew Berens

Dr. Matthew Berens earned bachelor's degrees in chemistry and biochemistry/molecular biology from Bethel University in St. Paul, Minn. (2015). As

an undergraduate student, Matthew used electron microscopy and advanced spectroscopic techniques to investigate the pore-scale structural features that influence nutrient adsorption in pyrogenic carbon materials. He also completed an internship with Medtronic (Minneapolis), evaluating the performance of ion-exchange resins for in-home kidney dialysis systems.

Matthew then received a PhD in civil engineering from the University of Minnesota in 2020. Under the advisement of Dr. William Arnold, his dissertation broadly explored themes regarding the fate and transport of organic pollutants in terrestrial and aquatic ecosystems. In collaboration with Eawag (Swiss Federal Institute of Aquatic Science and Technology), Matthew combined compound-specific isotope analysis with X-ray based characterization techniques to quantify and predict the reductive transformation of organic contaminants at redox-active mineral surfaces. He also partnered with multiple private, state, and federal research agencies to establish the first statewide monitoring program for neonicotinoid insecticides in aquatic systems in the state of Minnesota.

From 2021–2023, Matthew was a postdoctoral researcher at the University of Minnesota–Duluth Natural Resources Research Institute (NRRI). At NRRI, he combined basic and applied research to analyze the biogeochemical interactions of sulfur cycling and mercury methylation in mining-impacted wetlands, to create novel passive treatment systems for *in situ* environmental remediation. He also developed methods using high-resolution mass spectrometry to examine the relationship among the distribution of chemical and biological toxins and biogeochemical properties of sediments in the U.S. Great Lakes. In January 2023, Matthew began a postdoctoral appointment in the ORNL Environmental Sciences Division under the advisement of Dr. Elizabeth Herndon. At ORNL, he is working to investigate the biogeochemical controls on phosphorus cycling in coastal wetlands (Dr. Herndon DOE Early Career Award) and to evaluate how hydrologic gradients in non-perennial streams influence solute export from headwater catchments (WaDE SFA). Matthew's hobbies include hiking, reading, exploring and observing nature, and doing the New York Times Crossword puzzles.

Kristen Bidas

Kristen Bidas graduated with her bachelor's degree in chemistry from Stony Brook University in 2014. During her time as an undergraduate,

Kristen participated in a study abroad program that combined conducting oceanographic research with learning to sail a tall ship with Sea Education Association in Woods Hole, Mass. Her research project while aboard the SSV Robert C. Seamans involved collecting and counting microplastics in surface water and at depth in the North Pacific Subtropical Gyre. Before graduating, Kristen worked on a pilot study studying submarine groundwater in Jamaica Bay, N.Y., using $^{226}Ra/^{228}Ra$ radioisotopes by analyzing calcareous algae with gamma spectroscopy.

Kristen then earned her master's degree at Stony Brook University in chemical oceanography in 2017. Under the mentorship of Dr. Mary Scranton, Kristen studied elemental sulfur species in the Cariaco Basin (a sulfidic basin off the coast of Venezuela) using high-performance liquid chromatography (HPLC) and Raman microspectroscopy. She compared her results from the Cariaco Basin to a sulfidic lake in Fayetteville, N.Y. After graduation Kristen started working at Pace Analytical, an environmental laboratory in New York. There she analyzed contaminants in wastewater and drinking water using gas chromatography and HPLC.

In 2020 Kristen started her dissertation research under Dr. Elizabeth Herndon at the University of Tennessee and ORNL. Her dissertation research investigates carbon and manganese biogeochemical cycling in soils. This research involves coating sand with either manganese or iron oxides and incubating them in soil in a temperate forest in East Tennessee and tundra on the North Slope of Alaska. These mineral-coated sands have been analyzed using chemical extractions, synchrotron X-ray techniques, and neutron scattering. In addition, Kristen has taken soil cores and will use chemical extractions and synchrotron X-ray techniques to compare them to the mineral bag field experiments. Kristen's hobbies include traditional Japanese jujutsu, traditional Japanese swords, figure skating, pasta making, and seashell collecting.

Deandre Presswood

Deandre Presswood earned his bachelor's degree in environmental science from the University of Northern Iowa in 2021. Under the mentorship of Dr. Mohammad Z. Iqbal, Deandre used an ion chromatograph and suspended sediment analysis, in conjunction with classical field hydrology methods, to research the effects of stream discharge on mass transport of sediments and nutrients. While

simultaneously conducting hydrologic research, under the guidance of Dr. Alan Czarnetzki, Deandre researched atmospheric mixed-layer interactions. Using portable weather balloon systems, he captured high-resolution data of mixed-layer atmospheric conditions at varying altitudes above Cedar Falls, Iowa.

After graduation, Deandre worked for Colorado Springs Utilities in leak detection. By analyzing flow meters and using chemical baseflow separation along with acoustic monitoring, leaking infrastructure could be isolated and pinpointed for repair.

Deandre is pursuing his master's degree at Georgia State University in geosciences with a concentration in water science under the mentorship of Dr. Sarah H. Ledford. He is researching the effects of hydrologic disturbances across varying impervious surface cover in relation to stream metabolism using long-term continuous dissolved oxygen data and modeling packages such as streamMetabolizer. Deandre's hobbies include basketball, hiking, playing guitar, and exploring nature.

National and International Impact

ORNL WaDE SFA team members attend strategic conferences in the United States and abroad to gain insights into the state of the science, share project findings and strategies with the broader watershed and freshwater science research community, and identify collaborative opportunities. From November 2022 to June 2023, SFA scientists delivered or published 13 presentations, abstracts, or posters (see Appendix C, p. 22 for details). In this section, we highlight team members' contributions to the 2022 American Geophysical Union Fall Meeting, the 2023 Environmental System Science Principal Investigators Meeting, and the 2023 Gordon Research Conference on Catchment Science.

American Geophysical Union (AGU) Fall Meeting. Several SFA team members attended the AGU Fall Meeting in Chicago, Ill., on December 12–16, 2022. Saubhagya Rathore convened, and Marie Kurz, Scott Painter, and Adam Ward chaired the session, "Groundwater-Surface Water Interactions: Integrating Physical, Biological, and Chemical Patterns and Processes Across Systems and Scales." Other SFA team members also gave oral and poster presentations at the meeting.

BER's Environmental System Science Principal Investigators (PI) Meeting and Cyberinfrastructure Working Group Meeting. SFA members attended the PI Meeting from May 15–17, 2023, at the Hyatt Regency Bethesda in Bethesda, Md. SFA team members participated in the working group meeting, the plenary, and breakout sessions. Eric Pierce presented at the working group meeting. Elizabeth Herndon presented and served as panelist on the Early Career panel, and Jesus Gomez-Velez presented at the Remote Sensing/AI-ML/Crowdsourcing breakout.

Gordon Research Conference (GRC) on Catchment Science: Interactions of Hydrology, Biology, and Geochemistry. Marie Kurz, Scott Painter, and Saubhagya Rathore attended the GRC in Andover, N.H. on June 18–23, 2023. They each presented posters on new plans for the SFA and recent ATS advances.

Organizational Leadership and Collaborative Research Activities

Dr. Eric Pierce is the overall SFA program lead and is responsible for ensuring integration and success. He is the point of contact with BER Environmental System Science program managers and speaks to Paul Bayer biweekly on SFA progress and potential issues. Drs. Marie Kurz and Elizabeth Herndon serve in programmatic deputy roles to the PI and aid in planning and coordinating the project's overall scientific direction. The theme leaders and modeling activity lead—Drs. Elizabeth Herndon and Alex Johs for Theme 1, Dr. Scott Brooks for Theme 2, Drs. Marie Kurz and Natalie Griffiths for Theme 3, and Dr. Scott Painter for Crosscutting Modeling—are responsible for integrating activities within and across themes. Theme 1 will collaborate with Drs. Kamini Singha (Colorado School of Mines) and Holly Barnard (University of Colorado–Boulder). Dr. Singha will provide expertise in subsurface geophysics, and Dr. Barnard will provide expertise in how vegetation impacts stream dynamics. Dr. Erin Hotchkiss (Virginia Polytechnic Institute and State University) is an aquatic ecologist and biogeochemist with expertise in understanding how environmental change impacts biogeochemical processes in freshwater ecosystems. Dr. Hotchkiss will primarily support Theme 2 but will also engage in research activities being performed in Theme 3. Theme 3 will be performed in collaboration with Drs. Matt Cohen (University of Florida) and Adam Ward (Oregon State University). Drs. Cohen and Ward will respectively provide expertise in network-scale ecosystem metabolism and network-scale hydrology. Dr. Lydia Zeglin (Kansas State University) is a microbial ecologist with expertise in stream microbial diversity; her expertise will span across all three themes along with ORNL microbial expertise from Drs. Mircea Podar and Melissa Cregger. These theme leaders, along with the broader team, meet biweekly to provide an update on current research directions, future plans, and changes in staffing.

ORNL WaDE SFA Partners

Colorado School of Mines
University of Colorado Boulder
Virginia Tech
University of Florida
Oregon State University
Kansas State University

National Laboratory Investments

ORNL is committed institutionally to the success of the WaDE SFA program. In FY23, ORNL supported three Laboratory-Directed Research and Development projects and invested over $1 million in equipment and lab space upgrades in support of the WaDE SFA.

Appendix A. References Cited

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Santos, F., and E. Herndon. 2023. "Plant-soil relationships influence observed trends between Mn and C across biomes," *Global Biogeochemical Cycles* **37**(1), e2022GB007412. DOI:10.1029/2022GB007412.

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Appendix B. SFA Publications

See website for complete list (www.esd.ornl.gov/programs/rsfa/**).**

Manuscripts Published or In Press

Becker, P. S., A. S. Ward, S. P. Herzog, and S. M. Wondzell. 2023. “Testing hidden assumptions of representativeness in reach-scale studies of hyporheic exchange,” *Water Resources Research* **59**, e2022WR032718. DOI:10.1029/2022WR032718.

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Liang, X., A. Johs, M. J. Abernathy, J. Zhao, H. Du, P. Ku, L. Zhang, N. Zhu, X. Yin, S. C. Brooks, R. Sarangi, E. M. Pierce, and B. Gu. 2023. “High methylation potential of mercury with mixed thiolate ligands by *Geobacter sulfurreducens* PCA,” *Geochimica et Cosmochimica Acta* **342**, 74–83. DOI:10.1016/j.gca.2022.12.008.

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Santos, F., and E. Herndon. 2023. “Plant-soil relationships influence observed trends between Mn and C across biomes,” *Global Biogeochemical Cycles* **37**(1), e2022GB007412. DOI:10.1029/2022GB007412.

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Wood, D. L., K. A. Cole, E. M. Herndon, and D. M. Singer. 2023. "Lime slurry treatment of abandoned coal mine spoil: linking contaminant transport from the micrometer to pedon-scale," *Applied Geochemistry* **151**, 105617. DOI:10.1016/j.apgeochem.2023.105617.

Wymore, A. S., A. S. Ward, E. Wohl, and J. W. Harvey. 2023. "Viewing river corridors through the lens of critical zone science," *Frontiers in Water* **5**, 1147561. DOI:10.3389/frwa.2023.1147561.

Zhang, L., Y. Yin, Y. Sun, X. Liang, D. E. Graham, E. M. Pierce, F. E. Löffler, and B. Gu. 2023. "Inhibition of methylmercury and methane formation by nitrous oxide in Arctic tundra soil microcosms," *Environmental Science & Technology* **57**(14), 5655–65. DOI:10.1021/acs.est.2c09457.

Manuscripts In Review

Du, H., X. Yin, X. Gu, E. M. Pierce, and B. Gu. In revision. "Dissolved elemental mercury [Hg(0)aq] reactions and purgeability in the presence of organic and inorganic particulates," *Environmental Science & Technology Letters*.

Herndon, E., M. Newcomer, L. Ma, and A. Shiller. Submitted. "Trace elements and their isotopes in streams and rivers," invited book chapter in *Treatise on Geochemistry 3rd Edition: Hydrosphere.*

Herndon, E., J. Richardson, A. Carrell, E. Pierce, and D. Weston. In review. "Sulfur speciation in *Sphagnum* peat moss modified by mutualistic interactions with cyanobacteria," *New Phytologist.*

Horita, J., D. B. Watson, S. Toyoda, S. C. Brooks, O. Warr, B. Sherwood Lollar, M. E. Conrad, and N. Yoshida. In revision. "Coupled hydrogeochemical-microbial processes at an acid, radionuclide-contaminated site at the US DOE Oak Ridge Reservation, Tennessee: Implications for bioremediation and life under extreme conditions," *Geochimica et Cosmochimica Acta.*

Jamil, A., D. F. Rucker, D. Lu, H. Cao, S. Brooks, and K. C. Carroll. In revision. "Locating and characterizing subsurface targets with electrical resistivity by comparison of machine learning for geophysical arrays as alternatives to inverse modeling," *Journal of Applied Geophysics.*

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Montgomery, A., E. Herndon, C. Sims, and S. Jagadamma. In revision. "Manganese sources and rates impact plant Mn concentrations and soil Mn fractions," *Soil Science Society of America Journal.*

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Tang, W., X. Bai, Y. Zhou, C. Sonne, M. Wu, S. S. Lam, H. Hintelmann, C. P. J. Mitchell, A. Johs, B. Gu, L. Nunes, C. Liu, N. Feng, S. Yang, J. Rinklebe, Y. Lin, L. Chen, Y. Zhang, Y. Yang, J. Wang, S. Li, Q. Wu, Y. S. Ok, D. Xu, H. Li, X. X. Zhang, H. Ren, G. Jiang, Z. Chai, J. Zhao, Y. Gao, and H. Zhong. Submitted. "Novel demethylation pathway removes mercury from crops," *Nature Food*.

Data Products Released

Brooks, S. C., and K. A. Lowe. In preparation. [Data Set] East Fork Poplar Creek Discharge at Kilometer 5.4 Water Year 2021. ORNL Mercury Science Focus Area (SFA) Data Collection, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tennessee, USA.

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Appendix C. Presentations and Conferences

Becker, P. S., S. L. Painter, S. Rathore, and A. S. Ward. “Where and When is Including Underflow Important for Representing Denitrification in the Hyporheic Zone?” American Geophysical Union Conference, December 12–16, 2022. Chicago, Illinois.

Brooks, S. C., E. R. Hotchkiss, and E. M. Pierce. “Watershed Dynamics and Evolution Science Focus Area Theme 2: Stream Corridor Processes.” Environmental System Science Principal Investigator Meeting, May 16–17, 2023. Bethesda, Maryland.

Carroll, K. C., C.-H. Tsai, D. F. Rucker, S. C. Brooks, and T. R. Ginn. “Transient Storage Model Parameter Optimization Using the Simulated Annealing Method.” American Geophysical Union Conference, December 12–16, 2022. Chicago, Illinois.

Herndon, E., F. Santos, and H. Li. “Litter Transformation During Decomposition as a Function of Warming and Manganese Addition.” American Geophysical Union Conference, December 12–16, 2022. Chicago, Illinois.

Johs, A., E. Herndon, X. Gu, M. Podar, M. Cregger, K. Singha, Holly Barnard, M.J. Abernathy, R. Sarangi, A. A. DiSpirito, J. D. Semrau, and E. M. Pierce. “Watershed Dynamics and Evolution Science Focus Area Theme 1: Dynamic Headwaters.” Environmental System Science Principal Investigator Meeting, May 16–17, 2023. Bethesda, Maryland.

Kurz, M. J., E. M. Pierce, E. Herndon, S. Brooks, A. Johs, N. Griffiths, M. Cregger, M. Podar, H. Barnard, M. Cohen, E. Hotchkiss, K. Singha, A. Ward, and L. Zeglin. “Understanding the Role of Heterogeneous Land Cover and Hydrologic Regimes on Stream and Watershed Hydro-biogeochemical Function.” Gordon Research Conference on Catchment Science: Interactions of Hydrology, Biology, and Geochemistry. June 18–23, 2023. Andover, New Hampshire.

Kurz, M., N. Griffiths, M. Cohen, L. Zeglin, J. Gomez-Velez, D. Lu, S. Rathore, S. L. Painter, E. Herndon, S. Brooks, and E. M. Pierce. “Watershed Dynamics and Evolution Science Focus Area Theme 3: Network Function-Understanding the Role of Heterogeneous Land Cover and Hydrologic Regimes on Stream Hydro-Biogeochemical Function Within and Across Mid-Order Watersheds.” Environmental System Science Principal Investigator Meeting, May 16–17, 2023. Bethesda, Maryland.

Lu, D., S. L. Painter, N. Griffiths, and E. M. Pierce. “Uncertainty Quantification of Machine Learning Models to Improve Streamflow Prediction in Changing Climate and Environmental Conditions.” American Geophysical Union Conference, December 12–16, 2022. Chicago, Illinois.

Ogbughalu, O., S. C. Brooks, A. A. Carrell, B. Kristy, and M. Cregger. “Understanding Microbial Structure and Cross-kingdom Interactions in Response to Urbanization Across Aquatic Ecosystem.” American Geophysical Union Conference, December 12–16, 2022. Chicago, Illinois.

Painter, S. L., E. T. Coon, S. Bhanja, J. Gomez-Velez, P. V. V. Le, and S. Rathore. “High-resolution and multiscale process-based modeling of watershed hydrology and reactive transport with Amanzi-ATS.” Gordon Research Conference on Catchment Science: Interactions of Hydrology, Biology, and Geochemistry. June 18–23, 2023. Andover, New Hampshire.

Pierce, E. M., M. Kurz, E. Herndon, A. Johs, S.Brooks, N. Griffiths, S. L. Painter, S. Rathore, J.Gomez-Velez, Xin Gu, D. Lu, M. Podar, M.Cregger, K. Singha, H. Barnard, E. Hotchkiss, M. Cohen, L. Zeglin, and A. Ward. “Watershed Dynamics and Evolution Science Focus Area: Overview.” Environmental System Science Principal Investigator Meeting, May 16–17, 2023. Bethesda, Maryland.

Santos F., and E. Herndon. “Interactive Effects of Nitrogen and Manganese Availability and Temperature on Losses of Carbon and Nitrogen from Leaves.” American Geophysical Union Conference, December 12–16, 2022. Chicago, Illinois.

Rathore, S., Phong Le, S. L. Painter, and E. M. Pierce. “Watershed Dynamics and Evolution Science Focus Area Modeling Crosscut: Model-Data Integration Strategies for Stream Metabolism Studies.” Environmental System Science Principal Investigator Meeting, May 16–17, 2023. Bethesda, Maryland.

Acronyms and Abbreviations

AGU	American Geophysical Union
ATS	Advanced Terrestrial Simulator
BER	Biological and Environmental Research Program
DFT	density functional theory
DOE	U.S. Department of Energy
EFPC	East Fork Poplar Creek
ER	ecosystem respiration
ERT	electrical resistivity tomography
GPP	gross primary production
GRC	Gordon Research Conference
HPLC	high-performance liquid chromatography
HUC	hydrologic unit code
MCMC	Markov-Chain Monte Carlo
NEON	National Ecological Observatory Network
NHD	National Hydrography Dataset
NRRI	Natural Resources Research Institute
ORNL	Oak Ridge National Laboratory
PI	principal investigator
SFA	science focus area
SRB	sulfate-reducing bacteria
STIC	stream temperature, intermittency, and conductivity
TRB	Tennessee River Basin
WaDE	Watershed Dynamics and Evolution
WaSP	waterborne self-potential arrays
WRR	water resource region