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ORNL's Critical Interface Science Focus Area (CI-SFA): An Overview

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Developing a process-rich, predictive capability that integrates field, laboratory, and modeling studies of mercury fate and transformation dynamics across broad spatio-temporal scales in low-order streams is the overarching aim of the Critical Interfaces Science Focus Area (CI-SFA) at ORNL. The overarching aim will be accomplished over three successive 3-year phases. The **Phase I** focus is to **determine the fundamental mechanisms and environmental factors that control mercury biogeochemical transformations at key interfaces in terrestrial and aquatic ecosystems.**

Low-order freshwater streams, such as East Fork Poplar Creek (EFPC) (the project's representative use case), constitute nearly 90% of the total stream length in the United States and are the most frequently occurring stream type (>85%). Because of their low hydraulic radius (cross-sectional area and wetted perimeter) and low average water velocity, these stream systems have high water–sediment contact times, which promote in-stream biogeochemical interactions and exchange. Questions being addressed in **Phase I** of the CI-SFA plan include:

- What is the role of EFPC periphyton biofilms in Hg transformations? Which Hg-methylating microbial groups dominate in different EFPC ecosystem compartments?
- What are the key geochemical and biochemical variables and their interactions affecting Hg-DOM complexation, Hg-cell surface interactions, cellular uptake, and methylation?
- How do cell-cell interactions and microbial community metabolism influence net monomethyl mercury (MMHg) production? What is the native function of Hg-methylation gene pair *hgcAB*?
- Which metabolic pathway feeds into reactions involving HgcAB? What are the molecular-scale drivers that control the behavior of Hg-NOM complexation?

Accomplishments in 2016 include a series of recent publications that highlight the role of periphyton biofilms on net monomethyl mercury (MMHg) production in EFPC, the discovery of an iron-reducing bacterium *Geobacter bemidjiensis* Bem capable of both methylating Hg and degrading MMeHg, the design of *hgcAB* biomarkers, and first-of-a-kind measurements of Hg-DOM complexes present in EFPC that influence Hg bioavailability. In addition to these publications, new results collected include characterizing HgS aggregates isolated from EFPC soils, delineating the global proteomic profiles of *G. sulfurreducens* PCA after *hgcAB* gene deletion, elucidating the roles of thiol ligands in Hg cellular sorption and bioavailability, applying the *hgcAB* biomarkers to a range of environmental systems (e.g., EFPC and SPRUCE), probing the transformation mechanisms from dimethylmercury to MMHg with DFT, and developing a proto-type simulation tool to predict mercury fate and transformation in low-order streams. Although the CI-SFA uses Hg and EFPC as representative use cases, the information generated and the integrated multi-scale approach can be extended to the understanding of biogeochemical processes that affect fate, toxicity, and fluxes of nutrients and other trace metals and radionuclides in complex, heterogeneous, and multi-scale environmental systems.