

**ORNL SFA: Biogeochemical and Molecular Mechanisms Controlling Mercury Transformation at a Contaminated Site in Oak Ridge, Tennessee, USA**  
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Biogeochemical factors controlling mercury transformation and methylmercury production present a serious knowledge gap at the US Department of Energy Oak Ridge Reservation and many other contaminated sites globally. ORR field data show that reduction in waterborne Hg levels does not necessarily lead to a decrease of methylmercury in water or in fish. This observation suggests that at high Hg levels (often present at highly contaminated source areas), either methylmercury production is inhibited or demethylation significantly exceeds methylation. This presentation will provide an overview of the Science Focus Area (SFA) program at the Oak Ridge National Laboratory (ORNL) that combines molecular to field-scale chemical and microbiological studies to understand various biogeochemical factors that control the net production of methylmercury. The main objectives are to elucidate the rates, mechanisms and controls of abiotic and microbial processes affecting Hg speciation and transformation, to resolve the critical Hg precursors that are produced and subsequently methylated, and to develop and validate subcellular models to understand the biochemical and biophysical mechanisms of transformation between Hg species and methylmercury.

Historical data for Upper East Fork Poplar Creek at the Oak Ridge Reservation will be presented, and new data and geochemical modeling results from laboratory to field investigations will be summarized. This is the first year of a multidisciplinary research program in which laboratory and microcosm experiments will focus on the fundamental processes that control Hg speciation, reactivity and methylation using chemical, biomolecular, spectroscopic and stable isotope techniques. Preliminary data from field and laboratory studies will be presented, which examine microbial processes and geochemical controls such as dissolved organic matter, ionic species and photochemical reactions on Hg redox transformation, mechanisms, speciation, and bioavailability for Hg methylation.

Future effort will continue to employ functional genomics to determine key microbial groups that influence methylmercury production under varying geochemical conditions. Investigation of structure and dynamics at the molecular level will reveal mechanisms of regulation and the role of interactions between subcellular components. Molecular simulation will be applied to known demethylation processes to provide an atomic level detailed understanding of key reaction pathways, and will be extended to elucidate microbial methylation mechanisms identified by advanced genomic techniques. These studies will form the basis of understanding of the oxidation-reduction and methylation-demethylation transformations that determine the fate of Hg in sediment-water environments.