**Title:** EMSL: A DOE Office of Science User Facility for Environmental System Science Research

Nancy Hess[1]*, Chris Anderton[1], Pubudu Handakumbura[1], Jim Moran[1], and Tamas Varga[1]

[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA

***Contact:** nancy.hess@pnnl.gov

**BER Program:** Scientific User Facility

**Project:** EMSL

**Project Website:** http://www.emsl.pnl.gov/

Robust, predictive models of elemental cycling in terrestrial ecosystems and contaminant fate and transport in the subsurface require understanding that leads to identifying key microbial, biogeochemical, and hydrologic processes that control species reactivity and mobility across multiple spatial and temporal scales. Probing these dynamic processes at molecular scale provides mechanistic information to accurately represent these processes in computational reactive flow and transport models or community land models —an important goal of many Environmental System Science researchers who address the nation's environmental and energy challenges. Linking experimental and theoretical approaches from molecular to field scales requires the convergence of diverse experimental and computational techniques, plus collaboration with experts from multiple disciplines.

At EMSL, we provide expertise for scientific studies and discovery with our integrated experimental, computational, and modeling and simulation resources. A few hot areas of community research include understanding the chemical fate and mobility of contaminants in the biogeochemical environment; the role of microbial communities driving nutrient cycling in the rhizosphere; the speciation of metal ions and complexes on surfaces, in solution, or incorporated into mineral phases; unraveling the molecular messaging between microbes, plants, soil, and geochemistry; and investigating plants' molecular phenotypic responses to environmentally controlled stressors, including temperature, water availability, light cycles, and $CO_2$ levels.

We are expanding capabilities to couple computational resources with data generation for knowledge generation. We are also pairing metabolomics measurements with NWChem molecular dynamics simulations to achieve "standards-free" accurate identification of metabolites, thereby expanding the number and diversity of metabolites identified by mass spectrometry. Additionally, we are performing genomic sequence analysis and data mining to improve the depth of coverage from proteomics studies. Our extensive expertise in multi-scale reactive transport modeling spans the pore-to-basin scale. In particular, our modeling expertise encompasses experience with a diverse suite of software systems, including SPH and TETHYS for pore- scale simulation and PFLOTRAN, Amanzi, and eSTOMP for continuum-scale simulation.

Access to resources at EMSL for environmental and biological sciences is free of charge to the research community and granted through a peer-review proposal process (www.emsl.pnl.gov/emslweb/proposal-opportunities).