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EMSL: A DOE Scientific User Facility for Earth System Science Research

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

EMSL, a DOE national user facility in Richland WA, provides integrated experimental, computational, and modeling and simulation resources and expertise for scientific studies and discovery in Earth Systems Science to users free of charge. There are numerous capability sets that are particularly relevant for such research. I) Next generation imaging and surface characterization experimental capabilities can be used to provide the spatially resolved elemental analysis, oxidation state determination, chemical speciation, mineral identification, and microbe-mineral associations necessary for understanding the chemical fate and mobility of contaminants in the biogeochemical environment or microbial communities and nutrient cycling in the rhizosphere. II) Advanced spectroscopic capabilities are used for determining the speciation of metal ions and complexes on surfaces, in solution, or incorporated into mineral phases. III) A comprehensive suite of mass spectrometry platforms for proteomics/metabolomics, whole transcriptome analysis, gene expression profiling, small RNA analysis, novel transcript identification, and many genome- and epigenome-directed applications provide EMSL users extensive capabilities for unraveling the interplay between microbes, plants, soil, and geochemistry. IV) An integrated suite of capabilities to support research in subsurface flow and transport provide data from the micron to the intermediate scale. Experts assist users with pre-experiment modeling to hydraulic characterization, numerical modeling, and post-process analysis on custom-built flowcells. V) EMSL' s Plant Ecosystem Lab offers different types of plant growth facilities including Conviron walk-in rooms and Percival chambers. This allows growing and investigating plants under environmentally controlled conditions with defined temperature, humidity, light intensity, and CO_2 levels.

EMSL is expanding capabilities to couple computational resources with data generation: we are coupling 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 and we are performing genomic sequence analysis and data mining to improve the depth of coverage from proteomics studies. The extensive expertise at EMSL 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.