EMSL: A DOE Scientific User Facility for Terrestrial and Subsurface Science Research

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Robust, predictive models of elemental cycling and contaminant fate and transport in the subsurface require understanding and identification of key geochemical and biogeochemical reactions that control species reactivity and mobility at multiple scales. The ability to identify and adequately probe dynamic processes at the molecular to pore scale can provide information needed to accurately simulate these processes with computational models and incorporate them into reactive flow and transport models, an important goal of many Environmental System Sciences researchers who address the nation's environmental and energy challenges. Linking of experimental and theoretical information 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 and computational resources and expertise for scientific studies and discovery in subsurface biogeochemical research to users free of charge. There are numerous capability sets that are particularly relevant for biogeochemical 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. 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) Comprehensive quantitative proteomics/metabolomics platforms, whole transcriptome analysis platforms, platforms for 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 microbial communities 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. Users have access to experts who assist with all steps of the research process from pre-experiment modeling to hydraulic characterization, numerical modeling, and post-process analysis on custom-built flowcells.

RadEMSL, EMSL's radiochemistry annex, greatly expands the range of experimental capabilities for analysis of environmental samples contaminated with radionuclides, is now available to users. The new facility consists of approximately 6000 sq ft of lab space. The surface analysis-imaging suite contains FIB-SEM, TEM-EELS, SPM, XPS, and EMP. The Magnetic Resonance Facility houses 100 and 750 MHz wide-bore NMR spectrometers, with a wide range of specialized sample environments and nuclide probes, as well as an EPR spectrometer. The Radiochemistry Annex also houses sample preparation, solution chemistry and analytical tools including XRD and fluorescence capabilities. These capability sets together with NWChem, EMSL's premier computational modeling code, and a suite of other numerical models of fluid flow and biogeochemical reactions (at molecular, pore, core and ecosystem scales), enable users to address subsurface biogeochemical research challenges from both experimental and modeling vantage points.