EMSL

Capabilities Series

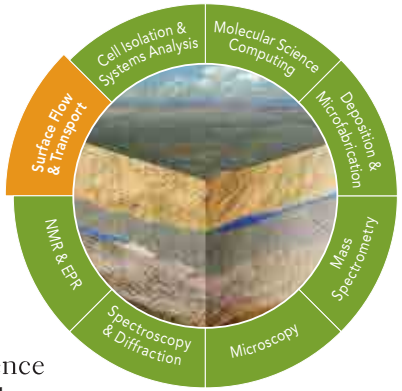
Subsurface Flow and Transport

From the micron scale to the geographic scale, EMSL houses an integrated suite of capabilities to support research and discovery in subsurface flow and transport. EMSL offers users access to cutting-edge instruments and the in-house support of experts, who assist with all steps of the research process from pre-experiment modeling to hydraulic characterization, analytical chemistry, numerical modeling, and post-process analysis.

When their integrated use is applied to EMSL's science themes of Biological Interactions and Dynamics, Geochemistry/Biogeochemistry and Subsurface Science, as well as Science of Interfacial Phenomena, subsurface flow and transport tools enable novel, fundamental research in:

- **Environmental contaminants** – tackling research in a holistic manner by integrating flow cells, analytical tools, and predictive modeling capabilities to study the fate and transport of contaminants, including metals, radionuclides, and chemicals
- **Predictive modeling** – understanding and predicting the behavior of subsurface contaminants
- **Environmental remediation** – providing public policy makers better information to make long-term remediation decisions.

CAPABILITY DETAIL



Micro Scale

- Clean-room capability for on-site fabrication of state-of-the-art micromodels for experimental work performed at EMSL
- Raman and epifluorescence microscopes with variable temperature/pressure

Intermediate Scale

- Wide variety of column, batch, radial, and rectangular flow cells
- Flow cells are used in coordination with high-precision, high-sensitivity analytical tools to generate data about sample characteristics, including the presence of carbon, trace metals, ions, nonvolatile compounds, thermally labile chemicals, and more

Instrumentation

- Capabilities include X-ray tomography; total organic analysis; dual-energy gamma scanning; and ion, liquid and gas chromatography

WHY USE EMSL'S SUBSURFACE FLOW AND TRANSPORT CAPABILITY?

- EMSL provides users the capability to focus on the application of fundamental physical chemistry concepts, and the study of chemical reactions in heterogeneous natural material – all with an emphasis on soil and subsurface systems.
- Users have the benefit of designing experiments using the predictive subsurface flow and transport simulator STOMP (Subsurface Transport Over Multiple Phases).
- Users have access to all other capabilities and experts at EMSL.

ABOUT EMSL

EMSL, a Department of Energy national scientific user facility located at Pacific Northwest National Laboratory, provides integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences to support the needs of DOE and the nation.

EMSL's distinctive focus on integrating computational and experimental capabilities, as well as collaborating among disciplines, yields a strong, synergistic scientific environment. Bringing together experts and an unparalleled collection of state-of-the-art instruments under one roof, EMSL has helped thousands of researchers use a multidisciplinary, collaborative approach to solve some of the most important and complex national scientific challenges in energy and environmental sciences.

To learn more about EMSL, the science conducted at EMSL, as well as the instruments and expertise available to users, www.emsl.pnnl.gov.

BECOME AN EMSL USER

Researchers are invited to access the world-class capabilities and collaborate with the internationally recognized experts at EMSL via its peer-reviewed proposal process. To submit a proposal, follow the five steps outlined on the EMSL website (www.emsl.pnnl.gov) under User Access. Current and potential EMSL users are encouraged to respond to Calls for Proposals, which are announced each spring. However, unique research proposals that fall outside the Calls for Proposal focus may be submitted at any time.

Applicants are encouraged to submit proposals for use of EMSL's capabilities with an emphasis on integrating computational and experimental tools. In general, most users whose open research proposals are accepted may use EMSL resources free of charge. Open research is loosely defined as science and engineering research for which the resulting information is published and shared broadly within the scientific community.

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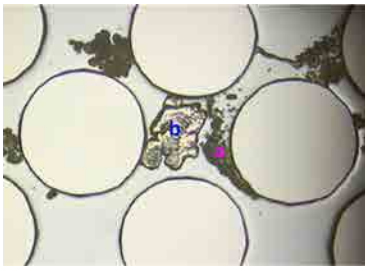
SSFT RESEARCH HIGHLIGHTS

Preventing Pollutants, Capturing Carbon



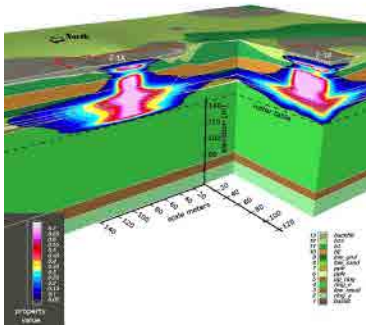
Small barricades of $CaCO_3$ form between simulated soil particles.

Cleaning up toxic materials in the groundwater relies on mixing different solutions to halt the pollutant's migration. The rapid formation of calcium carbonate ($CaCO_3$) could interfere with the mixing needed for remediation. EMSL users demonstrated how passages in the soil affect water flow and reactants mixing, as well as reverse the expected outcome of a common mineral precipitation reaction with implications for groundwater pollutants cleanup and geological carbon sequestration. The scientists studied solid $CaCO_3$ and showed that higher concentrations of the precursors for $CaCO_3$ result in less of the desired solid under dynamic flow and mixing conditions. This is because the solid forms in the passageways, or pores, and blocks further reactions. While this study did not directly address geologic carbon storage, the results could be beneficial to sequestration studies.

EMSL Users: PNNL and University of Illinois at Urbana-Champaign.

References: Zhang et al. 2010. *Environmental Science and Technology* 44:7833-7838.

Better Models, Better Remediation



Model predicting gaseous CCl_4 concentrations for two Hanford Site disposal areas (pink indicates highest CCl_4 levels).

Studies at EMSL demonstrate the importance of complex organic liquid mixtures in flow and transport models. The surface and interfacial tensions of liquids contaminating the environment are important because they affect the ability of those liquids to migrate in the subsurface. Basing experiments on a real-world scenario, EMSL users measured the surface and interfacial tensions of carbon tetrachloride- (CCl_4-) based nonaqueous-phase liquids and a wastewater solution. The research showed that in comparison to pure CCl_4, CCl_4-based mixtures had a significantly lower interfacial tension upon interacting with wastewater, increasing the speed and extent of contamination in the subsurface. Moreover, the properties and behavior of chemical mixtures need to be accounted for in models to provide accurate predictions and be most effectively used for remediation studies.

EMSL Users: University of Illinois at Urbana-Champaign and PNNL.

References: Nellis et al. 2009. *Vadose Zone Journal* 8(2):343–351.

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