# Role of Microenvironments and Transition Zones in Subsurface Reactive Contaminant Transport

**Pacific Northwest National Laboratory**
**Subsurface Science Scientific Focus Area (SFA)**

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## EXECUTIVE SUMMARY

The PNNL Scientific Focus Area (SFA) will resolve critical Hanford and basic subsurface science issues through integrated, multi-disciplinary, science-theme focused research on the role of microenvironments and transition zones in the reactive transport of technetium (Tc), uranium (U), and plutonium (Pu). Microenvironments are small domains within larger ones that exert a disproportionate influence on subsurface contaminant migration. They may be internal fractures or microbiologic niches within porous media lithic fragments; grain coatings, bio-films, or micro-colonies on larger mineral particles; or compact silt/clay stringers in gravel-dominated subsurface sediments. Transition zones are field scale features where chemical, physical, or microbiologic properties change dramatically over relatively short distances (e.g., ≤ 1 m). They exhibit steep, transport-controlled gradients of system controlling chemical species such as $O_2$, $H^+$, or organic carbon. Microenvironments and transition zones frequently dominate subsurface contaminant reactivity, with strong effects resulting from the coupling of chemical reaction, physical transport (advection, diffusion), and microbiologic processes. Past EMSP and NABIR research has documented the importance of these zones at the Hanford site.

The overall ten-year goals of the SFA are to develop: i.) an integrated conceptual model for microbial ecology in the Hanford subsurface and its influence on contaminant migration, ii.) a fundamental understanding of chemical reaction, biotransformation, and physical transport processes in microenvironments and transition zones, and iii.) quantitative biogeochemical reactive transport models for Tc, U, and Pu that integrate multi-process coupling at different spatial scales for field-scale application. Targeted contaminant chemical reaction and biotransformation processes include heterogeneous/biologic electron transfer, precipitation and dissolution, and surface complexation. The SFA will emphasize lab-based, coupled computational and experimental research using relevant physical/biologic models, and sediments and microbial isolates from various Hanford settings to explore molecular, microscopic, and macroscopic processes underlying field-scale contaminant migration. It will also pursue the refinement of geophysical techniques to define, characterize, and map spatial structures and reactive transport properties of microenvironments and transition zones in the field. The SFA will partner with the PNNL Environmental Molecular Sciences Laboratory (EMSL) to develop molecular understandings of key processes, and the Hanford Integrated Field Challenge (IFC) for access to, and samples from subsurface environments where these zones exist and are important.

The SFA will build on established areas of PNNL expertise in geochemistry, microbiology, and multi-scale modeling. Eleven individual, but highly collaborative research projects will focus on different scales, coupled processes, and/or contaminants; each will be managed by a

PNNL-ERSD investigator of significant accomplishment and appropriate expertise. The projects fall in the following science categories: i.) microbial ecology, ii.) molecular scale mechanisms, iii.) pore-scale coupled processes, iv.) reactive transport science, v.) multi-scale reactive transport models, and vi.) in-situ structures and reactive transport properties. An additional small project will also be established to mentor a promising new or young investigator. The PNNL team will be supplemented with 12 external, PNNL-supported investigators (lab, university) with needed complementary expertise. Cohesiveness and integration will be achieved by focus on SFA hypotheses formulated to enhance information upscaling, resolution of broader science issues, and Hanford impact. The overall SFA science program will be managed by two PNNL Chief Scientists who collectively have more than 40 years experience as BER PIs in subsurface biogeochemistry and contaminant fate and transport.