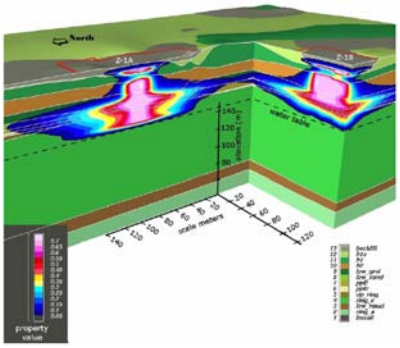
Mixing Things Up

Flow and transport models should account for fluid properties of complex mixtures

New results afforded by use of resources at the Department of Energy's EMSL demonstrate the importance of accounting for complex organic liquid mixtures in flow and transport models. Basing its experiments on a real-world scenario, a research team led by Professor Charlie Werth from the University of Illinois and involving participants from the Pacific Northwest National Laboratory measured the surface and interfacial tensions of carbon tetrachloride (CCl_4) based nonaqueous-phase liquids and a wastewater solution both composed of chemicals known to have been discharged at the DOE's Hanford Site in Richland, Washington. The surface and interfacial tensions of liquids contaminating the environment are of particular importance because they affect the ability of those solutions to migrate in the subsurface.



Modeling studies conducted by co-author Mart Oostrom to predict gaseous CCl_4 concentrations for two Hanford Site disposal areas show that simulations using the Werth team's data (above, pink indicates highest CCl_4 levels) yield larger contaminant plumes than simulations using single-component fluid properties.

For their experiments, the team prepared six CCl_4-based mixtures primarily containing tributyl phosphate, dibutyl butyl phosphonate, and lard oil as well as a representative wastewater solution containing nitrates and metals. In comparison to pure CCl_4, the CCl_4-based mixtures had a significantly lower interfacial tension upon interacting with wastewater; the surface tensions of the CCl_4-based mixtures compared to pure CCl_4 were minimally affected. The chemicals added to CCl_4 in solution also increased the mixtures' spreading coefficients such that if the mixtures were released to an uncontaminated area, they would spread quickly and contaminate larger areas of the subsurface than would pure CCl_4. Adding another complication, the mixtures change over time; for example, CCl_4 will volatize more quickly than the other components, leaving those components more concentrated in the mixture, thus lowering the mixture's interfacial tension. Per these results, the properties and behavior of chemical mixtures need to be accounted for in flow and transport models to provide accurate predictions and be most effectively used for remediation studies.

Scientific Impact: Real-world-based experiments such as these will lead to more enhanced fate and transport models for use by the remediation sciences and geochemistry communities. In addition, this work supports EMSL's goal to rapidly link theory with experiment.

Societal Impact: Models that incorporate data from real-world scenarios will predict the fate and transport of environmental contaminants more accurately, enabling the development of better remediation techniques and the protection of human health and the environment.

Reference: Nellis SR, H Yoon, CJ Werth, M Oostrom, and AJ Valocchi. 2009. "Surface and Interfacial Properties of Nonaqueous-Phase Liquid Mixtures Released to the Subsurface at the Hanford Site" *Vadose Zone Journal* 8(2):343–351.

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