Summary of 2006 Fall PI Meeting
Characterization and Modeling Discussion Section
October, 24 2006

Conveners:

David Lesmes (ERSP)
Todd Anderson (ERSP)

Presenters:

Graham Fogg (UCD)
David Lumley (4th Wave Imaging)
Ned Clayton (Schlumberger)
Susan Hubbard (LBNL)
Richelle Allen-King (Univ. of Buffalo/SUNY)
Tim Scheibe (PNNL)

Background

ERSP provides the fundamental science that serves as the basis for subsurface remediation needed across the DOE complex. To advance the understanding and simulation of subsurface processes that govern contaminant transport and remediation at the field scale, ERSP has solicited integrated field challenge proposals. Unlike most studies carried out by individual PIs (or small teams) to address a single question at a small spatial scale, the new field site(s) may provide an opportunity for multi-disciplinary team(s) of scientists to explore a range of integrated science questions over spatial scales that are relevant to DOE clean-up and LTM. Subsurface characterization and modeling components, which are needed to guide remedial treatments and validate the efficacy of the approaches in the presence of natural hydrogeological-biogeochemical heterogeneity, are likely to be integral components of the new field studies.

This session was designed to discuss issues of heterogeneity and the current state-of-the-practice associated with characterization and modeling at ERSP field research sites. Geophysical characterization and modeling approaches were then compared with the approaches used to explore petroleum reservoirs. The overall intent of the session was to explore if approaches used by the petroleum industry could be transferred for use at ERSP research field sites, and to identify outstanding characterization and modeling gaps that are unique to DOE contaminated aquifers.

Presentations

Graham Fogg (UCD) kicked off the characterization portion of the discussion section with a presentation entitled 'If heterogeneity is so important, why do we ignore it?' He described how assumptions about low variance in the log of hydraulic conductivity (lnK<2) permeate the literature (e.g., tables given by Gelhar, 1993 and Rubin, 2003). He argued that low lnK variance is actually rare, and that the unintentional misperception is largely due to the approaches that we use to measure K or to where we collect measurements. For example, well-test methods yield results that preferentially represent the high-K media, and often we preferentially sample in aquifers rather than in aquitards. Several examples were given that illustrated the significantly larger lnK variance associated with natural systems, including the LLNL site (alluvial system; ln-

K variance = 25) and the Wilcox aquifer system (interchannel sediments and channel-fill sands; variance = 18.9).

Graham emphasized how notions of homogeneity still permeate our conceptual and numerical models. This parsimony may stem from the misconceptions discussed above, but is also partially due to the difficulty and cost involved in characterizing subsurface variability. Because depositional facies exert a strong control on flow and transport properties, he suggested that improved characterization could be achieved through integration of measurements within a facies framework. This characterization could be performed using data collected from cores, geophysical logs, geological models, and geophysical data, and updated or verified using time-lapse hydrological-geochemical-geophysical measurements.

David Lumley (4th Wave Imaging) presented examples of approaches common for characterizing and monitoring petroleum reservoirs. He described how petroleum reservoir characterization is performed routinely, typically using a combination of extensive seismic and well log datasets, and how time-lapse seismic approaches are now commonly used for monitoring changes in reservoir pore fluids. Lumley also described approaches that are used to combine geophysical, hydrogeological, and production data to obtain a better model of the reservoir and its dynamics using, for example, stochastic approaches based on facies concepts and history matching techniques. An important message from David's talk was that even with the extensive datasets typically available for characterizing reservoirs, surprises are often encountered during drilling, and thus characterization should be viewed as an ongoing procedure that permits incorporation of updated information as it becomes available.

Ned Clayton (Schlumberger) provided more detailed information about the use of advanced well evaluation technologies in the petroleum industry. He described the decades of research that have been dedicated to developing methods to interpret wireline logs. Based on this research, the industry can now routinely use a vast array of logging tools to quantitatively estimate reservoir properties in the vicinity of the wellbore, such as lithology, pore fluid, and porosity. He also described recent advances in magnetic resonance imaging that can provide quantitative information about pore size distribution, bound versus free water, and permeability. Although reservoir conditions (temperature, pressure, degree of consolidation) are different from typical conditions associated with environmental studies, some of the tools that are used in the petroleum industry can also be used to characterize aquifer properties.

Susan Hubbard (LBNL) described characterization approaches associated with ERSP field study sites. She described how hydrogeophysical and biogeophysical methods have been successfully used to guide the choice of field study sites and sampling locations; to estimate fracture zonation, hydraulic conductivity, sediment geochemistry, and lithological zonation; to monitor amendment distribution and system transformation associated with remedial treatments; and to monitor changes in redox conditions important for sustained remediation. She described how the hydrogeological-biogeochemical information provided by the geophysical approaches has helped ERSP investigators to better design field studies and to interpret field experimental results.

Susan then compared the environmental and petroleum styles of characterizations. Susan illustrated how some of the components of ERSP-style characterization are similar to the

approaches used in the petroleum industry, such as the integration of multiple types of datasets using stochastic framework. She also outlined several differences that exist between environmental and petroleum approaches to characterization. For example, because the industry has recognized that understanding heterogeneity is a critical factor for their economic success, characterization is performed as a routine first step in petroleum exploration or development. Environmental projects, which are typically performed on smaller budgets, often view characterization as a luxury or tool to bring in when problems occur. Another primary difference is that environmental studies often require more information about biogeochemical properties than do petroleum studies. Susan suggested that although the environmental geophysical studies illustrate the potential that these methods have for improving our understanding of near subsubsurface systems, she emphasized that more research is needed to: perform quantitative characterization over larger spatial scales; better understand the relationship between geophysical attributes and biogeochemical properties; identify critical macroscale (field) properties and reaction rates, and understand how they relate to lab-scale measurements; and to develop better methods for routine integration and cataloguing of predictive models, characterization data, and information base across scales and sites.

Ned Clayton (Schlumberger) kicked off the modeling portion of the discussion section by briefly describing a petroleum industry approach to reservoir modeling using the Petrel framework. The workflow in this framework permits: integration of various datasets to generate the structural geometry of the reservoir; population of the geological layers with properties; upscaling of the properties to desired grid scales; predictions of reservoir responses using simulators and upscaled properties; post-simulation analysis; and updating as new information becomes available. Although many of these components are used for environmental work, the environmental community does not have a platform that allows input of various data, tools for integration and estimation (petrophysical modeling, facies modeling, etc.), and workflows to facilitate the use of disparate datasets for simulation and validation.

In addition to the importance of hydrogeological heterogeneity, **Richelle Allen-King** (SUNY Buffalo) emphasized the importance of understanding the impact of geochemical heterogeneity on contaminant transport processes. She described how geochemical data are typically even more limited than hydrogeological datasets, and she discussed the need to use rational methods to interpolate between point-based subsurface geochemical measurements using, for example, facies based approaches. She also emphasized the importance of identifying the rate controlling processes that are associated with particular environmental conditions and spatiotemporal scales of interest.

Tim Scheibe (PNNL) delivered the final talk of the session, which focused on the effects of heterogeneous coupled physical and biogeochemical processes across scales, where 'coupled processes' was defined as phenomena that act together to change the aquifer properties (such as the reduction in pore space and permeability brought about by changes in biomass or mineralization during biostimulation). He described how quantitative models of biogeochemical reaction systems, which are based on constituent concentration as the primary dependent variable, require assumptions that involve scales of averaging and mixing. He described how complete mixing and homogeneity conditions can be (and usually are) enforced at the laboratory scales, and that resulting theories are conditioned on those assumptions. However, at field scales,

he suggested that physical, chemical and biological heterogeneity and incomplete mixing are the rule rather than the exception. He then illustrated these concepts using several examples from ERSP research, including a combined field- and laboratory-scale study of bacterial transport, a field study of metals bioremediation in a highly heterogeneous aquifer, and pore- to continuum-scale simulations of coupled flow and mineral precipitation reactions. These examples demonstrated that 1) enhanced characterization (e.g., through high-resolution geophysics) can significantly improve model predictions, 2) proper representation of both physical and chemical heterogeneity is needed for reactive transport modeling, and 3) for the most challenging problems, it may be necessary to model some processes in extreme detail (e.g., pore-scale) which will require a new multi-scale modeling approach to be developed and implemented.

Open Discussion

After the characterization and modeling presentations, an open discussion ensued among meeting participants and speakers. Much of the conversation focused on exploring what characterization or modeling components should be undertaken at DOE sites; what has heretofore limited the implementation of these components; and if industry has tools or approaches that could be transferred for use at DOE field research sites. It was recognized that most of the DOE field research has been performed by small teams to address specific questions at the local scale (orders of meters). As such, the budgets are not sufficient to support components that were identified as important for field-scale remediation science, such as:

- **Scale issues**, including the development of techniques or understanding that permit the transfer of research results across laboratory - local field – plume field scales. Examples of science needs include the development of frameworks that permit rational integration of hydrogeological-geochemical-geophysical measurements. Although most of the conversation focused on geological or facies-based frameworks, other approaches (such as fractals) were also identified as potentially useful. Identifying rate-controlling processes at different scales was also identified as a critical gap – what are critical macroscale (field) properties and reaction rates, how do they relate to lab-scale measurements, and how can they be accurately characterized?

- **Modeling** issues, including the development, application, and verification of reactive transport models that can accurately predict processes across the pore to the plume scales, associated HPC needed to support such modeling, and the importance of incorporating uncertainty into the modeling effort.

- Development of advanced database-workflow-integration **tools** that link to predictive modeling systems. Such a system would permit easy cataloguing, integration, and visualization of collected data, facilitate collaborative team research, and permit use of acquired data for conceptual and numerical model development and hypothesis testing. The tools would easily allow the incorporation of new wells, time-lapse geophysical data, geochemical/isotopic datasets, hydrological forcing and other datasets as they become available, which would in turn permit updating of the conceptual or numerical models over time and by different investigators. As this concept is similar to the advanced geologically-based Schlumberger interpretation and 'living model' PETREL software

(http://www.slb.com/content/services/software/geo/petrel/index.asp), it was suggested that DOE could explore the use of this software for assisting ERSP projects.

- **Measurement** issues, including assessing the impact of measurement artifacts, biases, and uncertainty on remedial activities; the utility of geophysical approaches to assist with long term monitoring; and the importance of hydrological forcing to long term remedial treatments and stewardship.

Development of new ERSP research field site(s) offers the opportunity to bridge some of these gaps through strategic planning, coordination, and dedicated investments in characterization, modeling, and IT. Analogous to the 'infrastructure' associated with DOE user facilities, this investment would set the ERSD funded research sites apart from individual PI-led projects by providing the framework and tools needed to advance the science of field-scale remediation. Early activities associated with these sites might include, for example, the acquisition of 3-D geophysical data, advanced well-logs, and other hydrogeological-geochemical datasets that permit the development of a field-scale site conceptual model and framework that could guide subsequent sampling and intensive characterization efforts. Early efforts might also include the development (or adoption) of a site database and linked numerical modeling system that could permit hypothesis testing and updating as new datasets become available, and integration across local-scale efforts at the ERSD field research site(s).