A MESO-SCALE APPROACH ADDRESSING DOE SUBSURFACE ENVIRONMENTAL ISSUES: THE IDAHO NATIONAL ENGINEERING AND ENVIRONMENTAL LABORATORY SUBSURFACE SCIENCE INITIATIVE

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ABSTRACT

The Idaho National Engineering and Environmental Laboratory (INEEL) Subsurface Science Initiative is a multi-institutional, coordinated, interdisciplinary research program focused on the field-scale subsurface environmental research needs of the U.S. Department of Energy (DOE). The goal of the initiative is to develop new insights and improved understanding of processes occurring within the earth's subsurface, and to use this improved understanding to accurately predict and monitor the movements and transformations of contaminants. New insights and better understanding of subsurface processes will provide a sound technical basis for cost-effective cleanup solutions and improved long-term stewardship of DOE lands. The research agenda for the initiative is being developed through consideration of the science and technology needs identified in concert with subsurface problem holders from the INEEL and other DOE sites.

The Initiative is making extensive use of meso-scale experiments and field-scale observations. Meso-scale experiments are experiments using intact blocks retrieved from DOE field sites or engineered representations of the subsurface with controlled heterogeneity conducted at scales large enough to allow rigorous evaluation of the coupled field-relevant physical, chemical, and microbial processes influencing contaminant fate and transport. These complex experiments will result in improved modeling and monitoring tools and approaches that are critical components in improved decision making. In addition, meso-scale experiments can be used to 1) help distinguish between alternate field-based conceptual models of subsurface contaminant behavior, 2) evaluate the long-term performance of subsurface engineered solutions, and 3) conduct prototype and proof-of-principle testing. Initial research conducted through the Initiative is using observations and problems from contaminated INEEL sites to focus the design of the meso-scale experiments. Problems being considered include mixed waste landfills, contaminated vadose zones, mixed contaminant groundwater plumes, and contaminated soils. Because these problem sets are common across the DOE complex, tools and approaches developed through the Initiative will have applicability throughout the DOE complex.

INTRODUCTION

The Idaho National Engineering and Environmental Laboratory (INEEL) has undertaken a major research initiative in subsurface science to develop an improved understanding of processes occurring within the earth's subsurface. A better understanding of subsurface processes will be used to develop improved approaches and tools for 1) predicting the fate and transport of contaminants in the subsurface and 2) monitoring the distribution and movement of contaminants in the subsurface. The key element of the approach used in the Subsurface Science Initiative include:

- **Field oriented.** The subsurface environmental problems of the U.S. Department of Energy (DOE) occur at the field scale and require field-scale solutions. Historically, much of the environmental research has been conducted in traditional laboratory settings with little consideration of how the results would be translated to field applications. The Initiative will use field-scale issues to drive the research agenda.

- **Coordinated.** Much of the fundamental subsurface environmental research funded by the federal government consists of individual investigator-initiated projects. Although individual projects may provide outstanding research results, the full benefit of the collection of projects is not realized because the synergism among projects is not well developed. The Initiative will use its focus on field-scale issues to coordinate research activities.

- **Interdisciplinary.** Subsurface environmental research needs are by their nature interdisciplinary. The Initiative will use its focus on field-scale issues and approach to research to effectively identify and incorporate the needed disciplines (e.g., geology and geophysics, hydrology, geochemistry, microbiology, and modeling) into integrated interdisciplinary teams.

- **Multi-institutional.** No single institution has all the required expertise or facilities to address all subsurface environmental research needs. The Initiative will reach out to and team with other national laboratories, federal agencies, and the university research community to build a premier subsurface science research organization focused on DOE needs.

In addition, the Subsurface Science Initiative is problem oriented and is focused on the types of environmental remediation and stewardship issues that have resulted from DOE waste disposal practices. Problems being considered include mixed waste landfills, contaminated vadose zones, mixed contaminant groundwater plumes, and contaminated soils. Because these problem sets are common across the DOE complex, tools and approaches developed through the Initiative will have applicability throughout the DOE complex.

THE SUBSURFACE PROBLEM

The U.S. Department of Energy has conducted energy research, and weapons development and production at facilities in 31 states and in Puerto Rico. Toxic, radiologically contaminated, or mixed waste generated at these sites has been introduced into the underlying soils and aquifers because of a number of practices:

- Direct injection of waste into aquifers

- Discharge of wastewater into cribs and seepage basins

- Leakage from high-level waste underground storage tanks

- Leaching of contaminants from waste buried in trenches and pits.

At present, it is estimated that approximately 793 million cubic meters (Mm^3) of media at 132 sites have been, or are being, contaminated. Of this total, 97% are soils, underlying vadose zone materials, and groundwater. Groundwater represents about 89% (708 Mm^3) of the total media and includes 407 Mm^3 contaminated with organic waste, 291 Mm^3 contaminated with radioactive waste or mixed low-level radioactive waste, and 10 Mm^3 contaminated with nonradioactive inorganics or inorganic-organic mixtures [1]. Chlorinated solvents such as trichloroethene (TCE) were in widespread use throughout the DOE complex, and are the most common groundwater contaminants at DOE sites. In addition to contaminated groundwater, historical disposal practices have contaminated the vadose zones above aquifers. Although only 7% (58.5 Mm^3) [1] of contaminated media are in the vadose zone, they are of particular importance because the vadose zone is difficult to remediate and the contamination can be a continuing source of groundwater contaminant plumes.

Remediation of DOE lands is hampered by the lack of a comprehensive understanding of the processes occurring in the subsurface, for example, contaminant distribution and mobility. Subsurface contaminant migration has adversely impacted groundwater resources. Many of the technologies proposed for remediation or containment are ineffective or too costly. Improved methods for vadose zone plume characterization and data interpretation, new containment technologies, and innovative in situ remedial treatments are required to protect the nation's groundwater resources from contamination. In addition, as DOE cleanup strategies increasingly favor long-term in situ containment and stabilization, long-term stewardship responsibilities increase. These responsibilities require more robust subsurface characterization and monitoring methods, human health and ecological risk assessment approaches, and a better understanding of the long-term geologic processes affecting the sites. Key to developing these new methodologies and technologies is an enhanced understanding of the interdependent physical, geochemical, and biological processes as they are manifested in spatially and temporally heterogeneous subsurface environments, and a thorough comprehension of the regional context for each site. In summary, because DOE environmental and stewardship problems occur at the field scale, the problems ultimately will require field-scale understanding and solutions.

SCIENCE NEEDS

Currently the DOE Environmental Quality (EQ) research portfolio includes environmental remediation research valued at $58.8 million [2]. However, an analysis of the portfolio by the Strategic Laboratory Council concluded that environmental remediation and long-term stewardship are inadequately addressed by existing research [3]. This analysis finds that the EQ Portfolio is underinvested and recommends increased research in environmental restoration and long-term stewardship. High priority needs include [3]:

- An improved understanding of the fate and transport of contaminants in the subsurface in general and the vadose zone in particular, including improved characterization and modeling approaches

- Improved understanding of long-term performance and monitoring of *in situ* containment and stabilization techniques (including caps)

- Improved understanding of natural attenuation and the potential role of monitored natural attenuation as an assist or alternate to active remediation.

Additionally, long-term subsurface science and technology needs are being identified through activities such as the "Deficiencies in Vadose Zone Understanding at INEEL [4]," the Complex Wide Vadose Zone Road Map [5], and DOE's Long Term Stewardship Road Map (currently under development by INEEL). The complex-wide Site Technology Coordinating Groups (STCG's) identify and prioritize science and technology needs required to expedite cleanup of DOE sites [6]. A recurring issue in all the needs analyses is the requirement for a better understanding of vadose zone processes affecting fate and transport of contaminants. Although only 7% [1] of contaminated subsurface media are in the vadose zone, they are of particular importance because:

- Vadose zone contamination can be a continuing source of groundwater contaminant plumes

- Most radioactive or mixed low-level radioactive waste unique to DOE are buried in the vadose zone

- Vadose zone cleanup is expected to account for approximately half the total cost of remediation of DOE lands [1].

The National Academy of Sciences (NAS), at the request of the Environmental Management Science Program, assessed DOE's research needs in subsurface science [7]. The detailed NAS conclusions are consistent with those reported in the EQ portfolio analysis discussed above [3]. Recurring technical themes of the NAS assessment are: multidisciplinary approaches to problem solving, effective integration of data and results from multiple sources, consideration of DOE relevant contaminants and radionuclides, and a focus on field phenomena and translation of laboratory results to field applications. A key feature of the NAS analysis is the emphasis on conducting research at multiple scales and developing approaches that allow translation of laboratory-scale results into field-based investigations [7].

Based on an analysis of DOE's subsurface research needs, the INEEL Subsurface Science Initiative is initiating and conducting research to develop an improved understanding of 1) physical flow and transport of fluids (water, gas, and nonaqueous liquids) in complex heterogeneous subsurface matrices and 2) biogeochemical transformations that occur in pristine (e.g., down gradient from contaminant plumes) and contaminated subsurface environments. Although DOE has funded and continues to fund research in these areas, the INEEL is pursuing an alternate approach to this research.

MESO-SCALE TECHNICAL APPROACH

Fluid transport and biogeochemical transformations must be understood, characterized, and measured at the field-scale to solve DOE's environmental subsurface contamination problems. Past efforts to understand these processes at this scale have included field-scale experiments. These experiments have obvious relevance but their utility is limited because of the

- Inability to completely control boundary conditions and achieve satisfactory mass balances

- Difficulty in conducting replicate experiments because of local heterogeneities
- Limited range of parameters that can be evaluated (e.g., one geology and climatic regime)
- Regulatory restrictions on using real contaminants or genetically-engineered organisms
- High cost associated with site characterizations and individual experiments.

Traditional bench-scale experiments can overcome many of the limitations of field-scale experiments by allowing replicate experiments and the evaluation of wide ranges of parameters at comparatively low cost. However, the application of bench-scale results to field-scale problems is complicated by issues associated with physical, geochemical, and microbial heterogeneity, coupling of nonlinear processes, and upscaling. For these reasons, the INEEL Subsurface Science Initiative is pursuing an alternate approach to subsurface research that places a strong emphasis on the extensive use of meso-scale experiments[a] to understand the coupled nonlinear physical, chemical, and biological subsurface processes that control the movement and transformation of reactive contaminants and other constituents in heterogeneous, variably saturated subsurface media (vadose zone and aquifers). Meso-scale experiments serve a similar role in investigating subsurface processes that pilot-scale testing does in engineering by bridging the gap between and linking traditional laboratory experiments with field observations.

The INEEL hosted a workshop entitled "Subsurface Processes at the Meso-scale" on May 8 and 9, 2000 in Salt Lake City, Utah. The workshop was attended by 35 participants from DOE headquarters, 6 national laboratories, and 11 universities. The workshop was a forum to discuss the role of meso-scale methods in linking the information gained from laboratory research with the results of field observations to address field-scale subsurface issues. The workshop participants concurred that meso-scale experiments are critical to understand the complex coupled processes occuring in the subsurface, and that meso-scale experiments can bridge the gap between small, less complex laboratory experiments and large, extremely complex, and expensive field activities. The chief advantages of meso-scale experiments are the ability to:

- Conduct experiments at a scale larger than is possible with standard laboratory experiment to accurately portray and observe coupled processes and some individual processes
- Investigate greater spatial dimensions (e.g., 3-dimensional) than are possible at the laboratory scale, which are required to realistically observe processes and interactions
- Control and measure experimental variable and boundary conditions (including the nature and distribution of heterogeneities and "climatic" regimes) with greater accuracy than in the field
- Achieve more rigorous mass balances of contaminants and fluids than is possible at the field-scale
- Conduct replicate experiments and comparisons of alternate treatments in similarly constructed experiments

- Test hypotheses that are not possible at the field-scale because of the cost of materials, labor, waste disposal, regulatory issues, etc.

- Test scalability issues, such as the applicability of laboratory data and fundamental knowledge to the field-scale, the accuracy of laboratory-scale results used to generate models representing field-scale processes, and the importance of unanticipated processes when hypotheses are tested at larger scales

- Test and compare remediation technologies in controlled experiments that use hazardous materials, radionuclides, or genetically-engineered microorganisms

- Test new instruments under controlled conditions to ensure that they are fully functional and of the highest quality prior to implementation in the field

- Collect high-resolution detailed data sets needed for model development and testing.

Fig. 1 shows how the meso-scale approach fills an existing gap between detailed mechanistic laboratory investigations and field observations. Field observations and locations provide the basis for hypotheses and alternative conceptual models that can be more rigorously tested at the meso-scale using materials (both repacked and intact) from the field locations. The meso-scale experiments leads to validated process models through better quantification of subsurface processes and their representation in numerical models. These experiments can also be used to differentiate among competing conceptual models for a given field site or coupling of subsurface processes. The robustness of the validated process models can then be tested by comparison to new observation at a single field site or by existing observations at alternate field locations.

Meso-scale experiments are also important to identify essential processes that require traditional laboratory-scale investigation, and serve to focus that investigation. In some cases the importance of the essential processes may not have been appreciated prior to conducting the meso-scale experiment. Laboratory investigations provide fundamental mechanisms (e.g., equilibrium constants and biodegradation reaction mechanisms) of isolated processes as well as parameter measurements (e.g., reactive surface, porosity, and hydraulic conductivity) for the materials used in the meso-scale experiments. Because of their reliance on both field observations and laboratory results, meso-scale experiments link laboratory results and field observations to yield validated process models that are consistent with results of traditional single processes laboratory investigations and coupled process observations of field-scale phenomena. The validated processes models in turn will yield improved prediction of the movement of subsurface contamination needed to support DOE's complex-wide cleanup and environmental stewardship decisions.

The successful implementation of a meso-scale approach to address subsurface science requires a coordinated, interdisciplinary, multi-institutional approach. Participants at the Subsurface Processes at the Meso-scale workshop concurred that the optimal way to address subsurface science issues is to incorporate them into integrated sets of experiments or meso-scale campaigns that would include opportunities for collaboration among researchers in multiple disciplines and institutions. The concept of meso-scale campaigns is appealing because subsurface research inherently involves numerous disciplines (including biology, chemistry, physics, geology,

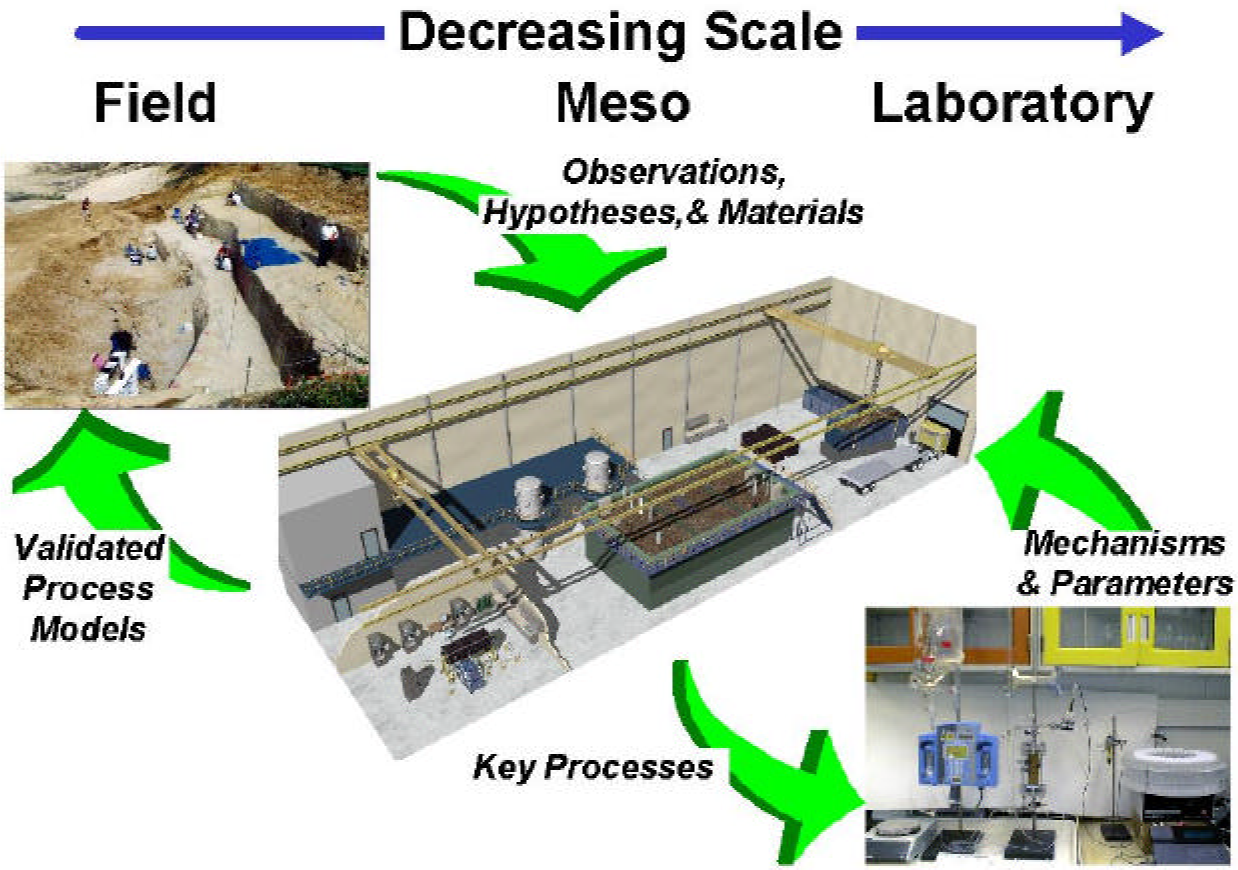

Fig. 1. The relationship between field-scale observations and laboratory-scale experiments and the role of meso-scale research in bridging the gap

A second, Subsurface Processes at the Meso-scale workshop is being planned for the spring of 2001. The goal of this workshop will be to design a meso-scale research campaign focused on a pressing DOE environmental need. Two examples of the types of campaigns envisioned are:

- Assessing effects of the degradation of co-disposed organics on vadose zone mobility of actinides at mixed waste landfills such as the Radioactive Waste Management Complex at INEEL. Specifically the campaign, through the use of meso-scale experiments, will elucidate the role of microbial produced carbon dioxide in the sorption and transport of actinides.

- Defining the rates of water and contaminant movement through the vadose zone at a site such as Idaho Nuclear Technology and Engineering Center. Specifically the campaign, through the use of geocentrifuge techniques and scaling theory, will assess the rates of water and colloid movement for varying infiltration scenarios (including engineered caps).

SUBSURFACE GEOSCIENCES LABORATORY

Meso-scale experimental campaigns require specialized facilities. As part of the Subsurface Science Initiative, the INEEL is developing plans for the construction of the Subsurface

Geosciences Laboratory (SGL). The SGL will be operated as a user facility and will house meso-scale research infrastructure, cutting-edge characterization capabilities, and state-of-the-art data management and visualization facilities necessary for analyzing the anticipated large volume of complex data collected in the meso-scale experimental campaigns. The meso-scale infrastructure is an essential aspect and a unique feature of the SGL to allow the following:

- Experiments that include 1) one-dimensional columns, 2) two-dimensional cells, 3) three-dimensional boxes (up to 1.8 × 3 × 2.5 m), 4) large tanks (up to 15 × 20 × 6 m), and 5) intact rock or soil/rock blocks (up to 1.5 × 1.5 × 1.5 m) excised from field sites

- Meso-scale test beds engineered and instrumented so that researchers can manipulate and measure biogeochemical reactions and mass transport phenomena in real time and with high four-dimensional resolution (e.g., space and time)

- The ability to readily modify the physical size (from sizes less than 10 m^3 to sizes exceeding 1,000 m^3) of meso-scale test beds to ensure maximum research effectiveness by focusing on the physical scale at which the process coupling mimics field conditions

- The ability to control boundary conditions, flow rates, temperature (including gradient and soil freezing), and atmosphere composition in multiphase meso-scale reactive flow and transport experiments

- Flexibility in real-time sensing and data acquisition of the appropriate physical, chemical, and microbial variables.

In addition to meso-scale research capabilities, the SGL will provide other specialized research infrastructure for DOE and INEEL's subsurface science research programs. The additional specialized infrastructure includes the following:

- A geocentrifuge for similitude modeling

- An engineered caps and barriers accelerated aging laboratory for model validation of caps and barrier performance

- High-speed data telemetry, high-speed network communications, and advanced data visualization

- A radiological laboratory for using beta and gamma emitters and transuranic (TRU)-type contaminants in multiphase fluid flow and biogeochemical transport experiments

- Mobile laboratories for collecting samples and retrieving intact blocks of soil and rock for laboratory experiments and for conducting meso-scale experiments at contaminated locations

EXPECTED RESULTS

The INEEL Subsurface Science Initiative with its focus on meso-scale research campaigns and the construction of the SGL will bring together the best technical minds with the state-of-the-science meso-scale research infrastructure to conduct subsurface science research addressing DOE's environmental needs. This research will provide DOE with 1) the scientific understanding of subsurface contaminant fate and transport and 2) the modeling and monitoring tools critical for defensible, cost-effective, and robust cleanup and long term stewardship decisions. Specifically, the research will provide:

- Superior simulation and visualization capabilities for predicting the transport and transformations of contaminants, allowing more realistic risk and performance assessments
- Accelerated deployment of new and existing *in situ* remediation technologies that minimize human exposure to contaminated media by virtue of treatment taking place underground, with minimal or no generation of secondary waste streams
- Enhanced vadose zone and groundwater monitoring systems that allow definitive evaluation of contaminant migration and the performance of engineered subsurface barriers
- An enhanced ability to design new, or improve existing, *in situ* remediation technologies that capitalize on the advancements made in fundamental understanding of geochemical and biological processes
- A science-based rationale for establishing cleanup levels that protect health and the environment and eliminate unnecessary remediation requirements for slightly contaminated subsurface media that pose minimal risk.

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FOOTNOTES

a. The meso-scale is defined as the intermediate physical and temporal experimental scale at which the coupling or interdependence of chemical, biological, and physical processes mimic the coupling that occurs under field conditions. The actual physical scale for a meso-scale experiment depends on the processes of interest and experimental objectives.