Need for a Subsurface Geosciences Laboratory as proposed by the Idaho National Engineering and Environmental Laboratory

Prepared by a Subcommittee of the Biological and Environmental Research Advisory Committee

April 2004

REPORT OF A SUBCOMMITTEE OF THE BIOLOGICAL AND ENVIRONMENTAL RESEARCH ADVISORY COMMITTEE ON THE NEED FOR A SUBSURFACE GEOSCIENCES LABORATORY, AS PROPOSED BY THE IDAHO NATIONAL ENGINEERING AND ENVIRONMENTAL LABORATORY

As part of its Subsurface Science Initiative (SSI), the Idaho National Engineering and Environmental Laboratory (INEEL) has proposed the construction of a specialized Subsurface Geosciences Laboratory (SGL). The SGL would house mesoscale experiments intended to link traditional laboratory experiments with field-scale observations. The SSI was begun while INEEL was under the management of the DOE Office of Environmental Management (EM), that component of the Department that is responsible for the decommissioning, decontamination, and remediation of the nuclear weapons processing and production sites. However, in 2003, management of the INEEL was transferred to the DOE Office of Nuclear Energy (NE), and NE has requested that the Office of Science conduct a review of the need for mesoscale experiments or facilities.

In July 2003, Dr. Raymond Orbach, Director of DOE's Office of Science (SC), charged the Biological and Environmental Research Advisory Committee (BERAC) with the evaluation of the proposed SGL. The charge letter to BERAC is found in Appendix A. The specific questions asked in that letter are:

- Is there a scientific need for the experiments at the mesoscale? What specific scientific issues require such experiments for their resolution? What are the advantages and limitations of mesoscale experiments? Are there alternative ways to achieve the same goals?
- What kind of experimental capabilities and facilities would be required to address these issues? Are there existing facilities with these or similar capabilities, and if so, what kind of results have they achieved.
- Will the facility being planned at INEEL be capable of addressing the scientific needs identified above? Are there plans in place for the operation and management of the facility? If so, are these plans appropriate and adequate?
- Is INEEL the appropriate site for the facility? Does INEEL have the appropriate scientific infrastructure (facilities, workforce, and related programmatic work) to support successful research at the facility?
- Would investing in this facility now be timely and appropriate for DOE? If not, is there a need for further assessment of the potential uses, limitations and strengths of the proposed facility compared to other existing or potential facilities?

In response to this charge, the Environmental Remediation Sciences subcommittee of BERAC convened a meeting on February 23, 2004. The participating membership of that subcommittee is found in Appendix B. The meeting involved formal presentations by experts in relevant scientific disciplines, both from INEEL and from academic institutions across the country. Subsequent to the presentations and interactive discussions between the scientific presenters and the BERAC subcommittee, the subcommittee met in executive session to formulate its recommendations. Staff members of the Environmental Remediation Sciences Division of the Office of Biological and Environmental Research were also present during the open session. The agenda for the meeting is found in Appendix C.

The agenda for the meeting was developed by Dr. Gill Geesey, liaison to the group proposing the SGL ("mesoscale facility"), in consultation with Dr. Michelle Broido, subcommittee chairman. Although preliminary architectural plans for the SGL had been developed when INEEL was under EM management, those plans had been focused on experiments that were directed specifically, and solely, to EM needs. With the change in management, the details of those plans became obsolete. Thus, Drs. Broido and Geesey agreed that the focus of the presentations and discussions would be on the scientific merit of a mesoscale facility, with very little discussion about design or operation of the facility. This limitation to the discussion is important, as reflected in recommendations found below.

The overall premise of the presentations was that for studies of fate and transport processes in the earth's subsurface, laboratory-based and field-scale experiments are often not sufficient for providing the kinds of detailed insights that are needed to understand and predict contaminant fate and transport processes in real subsurface systems. Although laboratory experiments are highly controlled and easily instrumented, they are idealized in terms of their small scale and composition, and they are rarely suitable for understanding coupled behavior in large or complex, heterogeneous environments. Field experiments, on the other hand, necessarily include the full complexity and scale of real environments but are limiting because they are difficult to fully control, instrument, monitor, and characterize. Mesoscale experiments offer an intermediate level for conducting experiments that focus on coupled processes in small and complex environments, yet that have greater degrees of control, instrumentation, monitoring, and characterization than are available in the field. In other words, the paradigm for subsurface research must be iteration between laboratory, mesoscale, field, and modeling experiments, and not simply between laboratory, field, and modeling experiments.

To bolster this premise, a number of examples were presented that documented the critical role that mesoscale experiments can play, are playing, or did play in developing the current understanding of subsurface phenomena. These not only included applications to environmental remediation, but applications to mining subsidence, carbon sequestration, the potential of methane hydrates as a future energy source, and oil field production were also presented.

Having discussed the importance of mesoscale experiments to these applications, the presenters then posited that a single facility housing several mesoscale experiments would have several benefits:

- There would be resident expertise in the construction of mesoscale experiments, including project management.

- There would be the establishment of, and interaction with, the complex databases necessary to record and organize the massive amount of data that would flow from each of the mesoscale experiments; similarly, facilities for visualization tools and model parameterization would be developed for broad use and access.

- Sophisticated instrumentation needed for different experiments could be shared, avoiding expensive duplication.

- With dedicated space for mesoscale experiments, these could be run for the long time periods that are often necessary without concern that the needed space would be confiscated for other purposes.

During its executive session, the subcommittee discussed the questions posed in Dr. Orbach's letter (Appendix A), and responses to those questions are presented below. Again, as noted above, there was very little either in the way of presentation or in the way of discussion about the design and operation of the proposed facility.

Is there a scientific need for the experiments at the mesoscale? What specific scientific issues require such experiments for their resolution? What are the advantages and limitations of mesoscale experiments? Are there alternative ways to achieve the same goals?

The subcommittee members were in agreement that there is substantial scientific merit in mesoscale experimentation, and it was felt that there would be similar consensus among members of the broader subsurface science research community. Indeed, mesoscale experiments have been conducted for years at a number of academic and government laboratories, both in the United States and in Europe. Mesoscale studies have been widely used to address research questions related to:

- Understanding and visualizing the impacts of physical, chemical, or microbial heterogeneities associated with real geologic media, on transport processes in multi-dimensional, multiphase flow systems (*e.g.*, in fractured vadose zone environments, current conceptual models of flow and transport are poorly developed).

- Assessing the impacts and influence of coupled (mathematically nonlinear) flow, transport, or reaction processes in multi-dimensional flow systems (*e.g.*, in the case of stimulation of bacteria to control subsurface redox for metal precipitation, there are complex issues about the coupled interactions between biomass growth,

mineral precipitation, nitrogen gas productions, permeability changes, and multidimensional flow).

- Determining how to scale understanding of flow, transport, or reaction processes, often expressed in terms in various conceptual and mathematical models, from the "laboratory" to the "field" scale.

- Establishing the viability and utility of new subsurface sensors and noninvasive imaging techniques.

In some instances, an important alternative to conducting mesocscale experiments is to carry out analogous “computer simulation experiments.” Numerical simulations in hypothetical, synthetically generated, or well characterized systems can be used to mimic physical experimentation and to study many of the same research questions cited above, including those related to assessing or scaling the impacts of heterogeneity and coupled processes on transport within multidimensional or multiphase flow systems. If applicable, computer simulation experiments offer some advantages over mesoscale experiments, such as greater control, better characterization, full access to all aspects of the solution, and faster experimental turnaround. Of course, they can also be limited in some very important respects, especially if the validity of the fundamental mathematical models upon which the simulations are based is uncertain.

That having been said, the subcommittee does not agree with the proposition that the paradigm for subsurface research must always be between laboratory, mesoscale, field, and modeling experiments. Rather, the inclusion of mesoscale experiments must come only when testing of an appropriate hypothesis requires such experiments. This will only be true for some subset of studies, not as a general rule. Further, the design and implementation of any mesoscale experiment is highly dependent upon the specific set of hypotheses being tested, and experience to date indicates that different scientific inquiries require dramatically different experiments.

What kind of experimental capabilities and facilities would be required to address these issues? Are there existing facilities with these or similar capabilities, and if so, what kind of results have they achieved.

Specific capabilities and facilities envisioned for the proposed SGL were not described or presented in any great detail. Nevertheless, representative kinds of mesoscale experiments carried out by INEEL personnel and their academic colleagues were discussed. One very valuable asset of the proposed SGL facility that was discussed is a recently-purchased experimental centrifuge that INEEL investigators, and their colleagues, are using to conduct scaled experiments related to fluid migration and mechanical deformation phenomena in partially saturated porous media.

During its deliberations, the subcommittee noted that mesoscale experiments have been developed and successfully conducted at many other locations (*e.g.*, Colorado School of Mines, Oregon Graduate Institute, Drexel University, University of Stuttgart, Pacific Northwest National Laboratory, and as part of the Yucca Mountain Project). Most of

these experimental facilities are limited in scope, often involving only one experimental apparatus, and many are relatively small in scale. They were typically developed by single or small numbers of investigators over relatively long periods of time, and they all have led to useful scientific results. Applications in these facilities have focused the assessment of effective transport behavior in heterogeneous media, visualization of the dynamics of non-aqueous phase liquids flow in unsaturated media, and characterization of the flow of water in partially saturated fractured rock. Again, however, the value of these experiments stems from their having been designed to test specific, if not unique, hypothesis.

Will the facility being planned at INEEL be capable of addressing the scientific needs identified above? Are there plans in place for the operation and management of the facility? If so, are these plans appropriate and adequate?

Is INEEL the appropriate site for the facility? Does INEEL have the appropriate scientific infrastructure (facilities, workforce, and related programmatic work) to support successful research at the facility?

INEEL has assembled an outstanding team of subsurface science researchers over the past several years. This team has both breadth and depth. INEEL is also establishing its reputation as a leader in studies of fractured vadose zone processes, and there are unique field capabilities associated with the Vadose Zone Research Park located at INEEL. INEEL would be an appropriate site for continued investment in studies of the vadose zone including, perhaps, a mesoscale facility of limited size that would foster intimate interplay between the mesoscale facility and vadose zone field studies at the site. Experience at the Field Research Center at Oak Ridge National Laboratory shows that mesoscale studies are often prompted by local field observations and that there can be very valuable synergy between field and mesoscale measurements.

Despite the strengths at INEEL, the subcommittee had serious reservations about the value of a large centralized facility as proposed. It is not likely that the needs of the community will be met by a facility having a few large flow tanks. It is more likely that each group of investigators will have need for a custom designed tank. A multi-scale facility that focuses upon physical heterogeneity may look quite different from one that emphasizes geochemical or microbiological processes. Again, since the specific hypothesis being tested will define the mesoscale experiment to be conducted, it is hard to envision a centralized facility. As pointed out both during the scientific presentations and during subsequent discussions, in many cases a mesoscale experiment will need to be operated for extended periods, often years. It was thus hard for the committee to visualize a facility that could accommodate both the diverse needs of multiple investigators and long term experiments for some subset of investigators.

As noted above, there was very little discussion about the details of the proposed facility other than it would be a centralized facility that could house multiple mesoscale experiments, would provide centralized information technology including databases, would provide centralized infrastructure such as machine shops and skilled personnel,

and would provide common monitoring equipment. There was no presentation on, or discussion about, the operation of this facility: how experiments would be prioritized, what would be supported by operating costs of the facility as opposed to the individual investigator, how long an experiment would be allowed to run, how many experiments could be supported at a given time, how experimental materials would be transported to the site, etc. Nevertheless, given the subcommittee's firm belief that mesoscale experiments must be hypothesis driven, it was hard to visualize a central facility that would be broadly applicable. For example, the subcommittee felt that the experimental set-up – the dimensions, slope, and linearity of the box (or other) to be used; the types, number, and location of monitoring ports; the materials to be used and the packing thereof – would need to be individualized to address the specific hypothesis. The subcommittee members could not envision the construction of multi-purpose set-ups that would have broad applicability. Similarly, given the discussions that some mesoscale experiments would need to be conducted over extended time periods, the availability for use by a broad community would be significantly curtailed.

Would investing in this facility now be timely and appropriate for DOE? If not, is there a need for further assessment of the potential uses, limitations and strengths of the proposed facility compared to other existing or potential facilities?

Mesoscale experiments have the potential to contribute valuable knowledge that support a number of DOE missions and offices. Applications to carbon sequestration support the DOE Office of Science, Office of Fossil Energy (FE), and Office of Energy Efficiency and Renewable Energy (EE). Applications to methane hydrates support FE and EE. Mining subsidence issues support FE. Understanding the vadose zone has important ramifications for both EM and NE, the former with regard to environmental contamination that has already occurred and the later with regard to potential environmental consideration should there be in a significant increase in the use of nuclear energy in this country. The scientific staff at INEEL and their collaborating partners are highly qualified to conduct valuable mesoscale research, and there is definite value derived from development of a common, shared infrastructure of facilities, equipment, sensors, and expertise. Nevertheless, the subcommittee cannot recommend the development of a centralized facility that would try to meet the needs of a diverse set of scientific inquiries.

APPENDIX A - CHARGE LETTER

Department of Energy
Office of Science
Washington, DC 20585

July 23, 2003

Office of the Director

Dr. Keith O. Hodgson
Director, Stanford Synchrotron Radiation Laboratory
Department of Chemistry
Stanford University
Stanford, CA 94305

Dear Dr. Keith Hodgson:

As part of the Idaho National Engineering and Environmental Laboratory's (INEEL) Subsurface Science Initiative (SSI), a major research undertaking aimed at expanding the understanding of subsurface contaminant fate and transport, INEEL has proposed the construction of a specialized Subsurface Geosciences Laboratory (SGL). The SGL would house mesoscale experiments intended to link traditional laboratory experiments with field-scale observations. The mesoscale experiments would be conducted at scales large enough to allow evaluation of the field-relevant coupled processes.

The SSI and SGL were initiated at the time that INEEL was designated as the "Lead Laboratory" for the DOE Office of Environmental Management (EM), and that Office was responsible for management of INEEL. In FY 2003, management of the INEEL was transferred to the DOE Office of Nuclear Energy (NE), and NE has requested that the Office of Science conduct a review of the need for mesoscale experiments or facilities.

To assist us in this assignment, I am asking the Biological and Environmental Research Advisory Committee to organize and oversee a review of the scientific basis and need for the proposed SGL facility. More specifically, the review should address the following questions:

- Is there a scientific need for the experiments at the mesoscale? What specific scientific issues require such experiments for their resolution? What are the advantages and limitations of mesoscale experiments? Are there alternative ways to achieve the same goals?
- What kind of experimental capabilities and facilities would be required to address these issues? Are there existing facilities with these or similar capabilities, and if so, what kind of results have they achieved.

- Will the facility being planned at INEEL be capable of addressing the scientific needs identified above? Are there plans in place for the operation and management of the facility? If so, are these plans appropriate and adequate?
- Is INEEL the appropriate site for the facility? Does INEEL have the appropriate scientific infrastructure (facilities, workforce, and related programmatic work) to support successful research at the facility?

  Would investing in this facility now be timely and appropriate for DOE? If not, is there a need for further assessment of the potential uses, limitations and strengths of the proposed facility compared to other existing or potential facilities?

I would like the review to be conducted in late January 2004, with a draft report to me by April 1, 2004. I would like to have a final report from BERAC prior to but no later than the Committee's Spring meeting.

Thank you and your Committee for your continuing help and support in advising the DOE on its research directions and plans.

Sincerely,

Raymond L. Orbach
Director

APPENDIX B
SUBCOMMITTEE ROSTER

Dr. Michelle S. Broido, Chairman, BERAC Member
Associate Vice Chancellor for Basic Biomedical Research
and Director, Office of Research, Health Sciences
University of Pittsburgh
Scaife Hall, Suite 401
3550 Terrace Street
Pittsburgh, PA 15261
mbroido@hs.pitt.edu
412-648-2232 (phone)
412-648-2741 (fax)

Dr. Richelle Allen-King (*ad hoc*)
Department of Geology
State University of New York at Buffalo
Department of Geology
876 Natural Science Complex
Buffalo, NY 14260
richelle@geology.buffalo.edu
716-645-6800 x3963 (phone)
716-645-3999

Dr. Margaret Cavanaugh
Office of the Director
Room 1205N
National Science Foundation
4201 Wilson Boulevard
Arlington, VA 22230
mcavanau@nsf.gov
703-292-8002 (phone)
703-292-9232 (fax)

Dr. Mark Rivers
Associate Director / GSECARS
9700 South Cass Avenue, Bldg. 434A
Argonne, IL 60439
rivers@cars.uchicago.edu
630-252-0422 (phone)
630-252- 0436 (fax)

Dr. Andrew F. B. Tompson
Environmental Science Division, L-208
Lawrence Livermore National Laboratory
PO Box 808
Livermore, CA 94551
afbt@llnl.gov
925-422-6348 (phone)
925 422-3925 (fax)

Dr. Samuel J. Traina
Director
Sierra Nevada Research Institute
University of California, Merced
P.O. Box 2039
Merced, CA 95344
straina@ucmerced.edu
209-724-4400 (phone)
209-724.4424 (fax)

Dr. Albert J. Valocchi (*ad hoc*)
Department of Civil & Environmental Engineering
University of Illinois at Urbana-Champaign
205 N. Mathews Ave.
Urbana, IL 61801
valocchi@uiuc.edu
217-333-3176 (phone)
217-333-0687 (fax)

AGENDA
Mesoscale Facilities Review

Date: February 23, 2004
Location: Latham Hotel Georgetown, 3000 M St. NW, Washington, D.C.

8:00 am Dr. Russ Hertzog, Director, INEEL Subsurface Science Initiative.

Introductions
Overview of the day's activities
Vision
Purpose of the Review
Concept

8:20 Presentations by representatives of the subsurface science community

Professor Gill Geesey, Montana State University, "A need for new experimental facilities for subsurface research at the mesoscale"

8:40 Professor Michael Silevitch, Director, NSF Center for Subsurface Sensing and Imaging Systems, Northeastern University. "A top down rationale for mesoscale facilities development"

9:10 Discussion

9:20 Professor Mary Wheeler, University of Texas. "Modeling coupled processes: A case for establishing a mesoscale subsurface experimental facility"

9:50 Discussion

10:00 Break

10:15 Professor T.C. Onstott, Princeton University. "What we need to learn about biogeochemical processes from mesoscale research"

10:45 Discussion

10:55 Professor Jack Istok, Oregon State University. "How a facility to conduct experimentation at an intermediate scale could complement field research activities"

11:25 Discussion

11:45 Professor Gill Geesey "Morning session wrap-up"

12:00pm Break/ Working Lunch

12:15 Presentations by INEEL scientists

Dr. Russ Hertzog, Director, INEEL Subsurface Science Initiative. “Mesoscale experimental research”.

12:30 Discussion

12:40 Dr. Robert Lenhard, INEEL. "Larger-Scale Experiments: Test our understanding of multiphase flow"

12:55 Discussion

1:05 Dr. Paul Meakin, INEEL. “Physical and computer modeling of multiphase flow in the fractured subsurface”

1:20 Discussion

1:30 Dr. Rick Colwell, INEEL. “Methane hydrate research requiring mesoscale experiments”

1:45 Discussion

1:55 Dr. Russ Hertzog, INEEL. “Why INEEL??

2:15 Discussion

3:00 Discussion and recommendations (Review Panel only)