Office of Science
Notice DE-FG01-05ER05-12

Environmental Management Science Program (EMSP): Transport of Contaminants in Subsurface Environments at DOE Sites

Department of Energy

Office of Science Financial Assistance Program Notice DE-FG01-05ER05-12: Environmental Management Science Program (EMSP): Transport of Contaminants in Subsurface Environments at DOE Sites

AGENCY: U.S. Department of Energy

ACTION: Notice inviting grant applications.

SUMMARY: The Office of Science (SC), U.S. Department of Energy (DOE), hereby announces interest in receiving applications for research grants in the Environmental Management Science Program (EMSP) to support innovative, fundamental research investigating coupled reactive contaminant transport processes across different spatial scales in heterogeneous subsurface environments at DOE sites; research is also invited on new tools for measuring subsurface properties and parameters important to understanding coupling and scaling phenomena.

DATES: Researchers are strongly encouraged to submit a preapplication for programmatic review. Preapplications should be submitted by February 10, 2005, to allow sufficient time for review of programmatic relevance and for subsequent preparation of the full application. The preapplication narrative of no more than two pages should consist of a description of the research objectives, approach, and relevance to DOE needs. The preapplication should also include a list of the key investigators, their disciplines and their institutions using at most one page.

The deadline for receipt of formal applications is 4:30 P.M., Eastern Time, Tuesday, April 26, 2005, in order to be accepted for merit review and to permit timely consideration for award early in Fiscal Year 2006.

ADDRESSES: Preapplications referencing Program Notice DE-FG01-05ER05-12 should be sent by E-mail to roland.hirsch@science.doe.gov.

Formal applications referencing Program Notice DE-FG01-05ER05-12, must be sent electronically by an authorized institutional business official through DOE's Industry Interactive Procurement System (IIPS) at: http://e-center.doe.gov (see also http://www.science.doe.gov/grants/). IIPS provides for the posting of solicitations and receipt of applications in a paperless environment via the Internet. In order to submit applications through IIPS your business official will need to register at the IIPS website. **IIPS offers the option of**

using multiple files, please limit submissions to one volume and one file if possible, with a maximum of no more than four PDF files. The Office of Science will include attachments as part of this notice that provide the appropriate forms in PDF fillable format that are to be submitted through IIPS. Color images should be submitted in IIPS as a separate file in PDF format and identified as such. These images should be kept to a minimum due to the limitations of reproducing them. They should be numbered and referred to in the body of the technical scientific grant application as Color image 1, Color image 2, etc. Questions regarding the operation of IIPS may be e-mailed to the IIPS help desk at: HelpDesk@pr.doe.gov or you may call the help desk at (800) 683-0751. Further information on the use of IIPS by the Office of Science is available at: http://www.science.doe.gov/grants/IIPS-Instructions.html.

If you are unable to submit an application through IIPS, please contact the Grants and Contracts Division, Office of Science at: (301) 903-5212 or (301) 903-3064, in order to gain assistance for submission through IIPS or to receive special approval and instructions on how to submit printed applications.

FOR FURTHER INFORMATION CONTACT: Dr. Roland F. Hirsch, Environmental Remediation Sciences Division, SC-75/Germantown Building, Office of Biological and Environmental Research, Office of Science, U.S. Department of Energy, 1000 Independence Ave., SW, Washington, D.C. 20585-1290, telephone: (301) 903-9009, E-mail: roland.hirsch@science.doe.gov, fax: (301) 903-4154. Please do not use regular mail as delivery may be delayed. The full text of Program Notice DE-FG01-05ER05-12 is available via the Internet using the following web site address: http://www.science.doe.gov/grants/.

SUPPLEMENTARY INFORMATION:

The Office of Science sponsors environmental remediation research to help fulfill DOE's continuing commitment to the cleanup of the Department's environmental contamination legacy. Proposed basic research under this announcement should contribute to environmental management activities that would decrease risk for the public and workers, provide opportunities for major cost reductions, reduce time required to achieve DOE's mission goals, provide contingency strategies, and, in general, should address problems that are considered to be intractable without new knowledge.

Program Funding

It is anticipated that up to a total of $4 million of Fiscal Year 2006 Federal funds will be available for new and renewal awards resulting from this Announcement. An additional sum, up to $4 million, will be available for competition by DOE National Laboratories under a separate solicitation (Program Announcement LAB 05-12). Three-year funding of awards is anticipated, contingent upon the availability of appropriated funds and successful annual progress. Award sizes will be determined by the scope and collaborative nature of the project. Collaborative projects involving several research groups or more than one institution conducting integrated research at multiple scales may be funded up to a limit of $600,000 per year over the three year cycle of the project. Single investigator projects should not exceed $400,000 per year over the three year cycle.

Investigators early in their careers and/or new to DOE's environmental remediation research program are encouraged to apply. The Program Manager is available to discuss new ideas and their alignment with the program.

Collaboration and Training

Multi-disciplinary and inter-institutional collaborations are strongly encouraged to enhance and strengthen research capabilities as needed. Collaboration could include institutions such as universities, industry, non-profit organizations, federal laboratories and Federally Funded Research and Development Centers, including the DOE National Laboratories. All applications should include letters of agreement to collaborate from included collaborators; these letters should specify the contributions the collaborators intend to make if the application is accepted and funded and outline a management structure for integrating collaborating investigators. DOE may encourage collaboration among prospective investigators by promoting joint applications or joint research projects based on review of the preapplications or through other forms of communication. Involvement of students and post doctoral scientists is encouraged. Refer to http://www.science.doe.gov/grants/Colab.html for details.

Representative Research Areas

Basic research is solicited to elucidate the influence of coupled biological, chemical and hydrologic processes on subsurface contaminant behavior at multiple scales in the vadose and saturated zones (including regions of saturated zone/surface water interaction) and for new tools and approaches that could be incorporated into this research to quantitatively assess process coupling and scaling in heterogeneous environments. Inherent in these studies is the need for multidisciplinary and integrated approaches that allow derivation and scaling of constitutive properties and development of conceptual and numeric models that describe reactive transport behavior in different hydrogeologic environments. Relevant scientific disciplines include, but are not limited to: geosciences (including geology, mineralogy, geochemistry, geophysics, hydrogeologic flow and transport modeling, process modeling, and hydrologic field-studies), chemical sciences (including fundamental interfacial chemistry, computational chemistry, actinide chemistry, and analytical chemistry and instrumentation), biological sciences (including microbiology and biogeochemistry), and engineering and materials sciences (including barrier systems design, diagnostics and transport processes).

Relevance to Mission

A key consideration in the evaluation of research applications will be applicability to the Environmental Remediation Science Division (ERSD) mission of DOE environmental remediation. Applicants will need to identify specific areas of scientific need and make a strong case for the value of the proposed research in helping resolve those needs. The application should explain how resolution of these needs could improve capabilities in site stewardship and/or contaminant remediation. Therefore, **all applications submitted in response to this Notice must explicitly state how the proposed research will support the accomplishment of the BER Long Term Measure of Scientific Advancement to develop science-based solutions for cleanup and long-term monitoring of DOE contaminated sites.**

DOE will also consider, as part of the evaluation, program policy factors including balance among the program areas and research already in progress. Past research solicitations, abstracts, and research reports of projects funded under EMSP can be viewed at: http://emsp.em.doe.gov/researcher.htm.

Subsurface Contamination Research Needs

The Department of Energy is responsible for remediation of waste and environmental contamination resulting from the nation's nuclear weapons program. The nuclear weapons complex includes 5000 facilities at 16 major sites and over 100 smaller sites located in a wide range of climatic and geologic conditions.

Research has been funded in this program to address a broad range of cleanup issues, ranging from facilities deactivation and decommissioning to health and ecological risk, but one of the most vexing problems has been how to identify, predict and control contaminant migration at DOE sites across the nation. The ability to define and predict contaminant transport will be critical to assess risk and, where needed, to develop innovative remediation methods to attenuate or remove contaminants. The need to predict contaminant mobility over the long-term is reinforced by DOE estimates that over 100 sites will have residual contamination once cleanup programs are completed (Reference: DOE, 2001b).

An assessment by the National Research Council of research needs in subsurface science at contaminated DOE sites (NRC, 2000a) explicitly recognized that contamination will remain in the subsurface after surface cleanup and that prediction of contaminant transport in conjunction with development of technologies for containment and stabilization of contaminants in-place are, and will continue to be, critical issues. Key needs in site stewardship that were identified include predicting and simulating the fate and transport of contaminants, developing appropriate remediation or stabilization methods based on this knowledge, and assessing performance of both predictive models and mitigation efforts over the long term.

The development of conceptual and numeric models for the fate and transport of contaminants is of primary concern to DOE ERSD as well as to the environmental science community. The inherent complexity of the subsurface in conjunction with the limited ability to observe processes and interactions as they occur in these systems has proven to be a major obstacle to predictive simulation of contaminant behavior at the field scale. A comprehensive DOE/SC effort to identify the technical frontiers in large scale simulation (DOE, 2004) called for interdisciplinary laboratory and field investigations of subsurface processes at all fundamental length scales. These advances in computation and modeling will reliably extend fundamental knowledge of the processes controlling contaminant reactivity at the molecular/microscopic scales to prediction of contaminant transport at the field. A recent assessment by an Interagency Steering Committee on Multimedia Environmental Models (ISCMEM, http://www.iscmem.org/) indicated that most of the ten participating agencies have programs to simulate the transport of chemical contaminants in subsurface environments. The assessment indicated that the most important technical issues facing the application of these simulations were (1) the formulation of coupled reactive process conceptual models representing a scientific understanding of processes controlling the transformation and movement of contaminants and other relevant properties and processes for a

specific system, and (2) how to scale reaction parameters for field scale simulation. Conceptual models should include the coupled reaction networks, hydrologic properties, and geologic structure for a specific system. Depending on the system, a conceptual model for a groundwater contaminant plume might also consist of descriptions of the spatial distribution of chemical and biological components; sediment and mineralogical properties; hydrologic properties, such as hydraulic conductivity; aqueous composition and controlling chemical and microbial reactions. (Davis et al, 2004)

A workshop was convened by the ISCMEM in 2004 to assess the state of the art in modeling processes controlling the field scale migration of contaminants and in conceptual model development and parameterization for reactive transport modeling. Research priorities were established and are summarized in detail (Davis et al, 2004) and the document is available on the Interagency Steering group web site (http://www.iscmem.org/). It was concluded that a major difficulty in conceptual model development is the identification of appropriate process models in the presence of multi-scale heterogeneities. It was further concluded that process and parameter upscaling in multidimensional systems can best be examined by studying transitions in system behavior across a range of scales. Investigation of conceptual models for inter-scale processes in the same system was thought to be the best approach to identify independent constraints on the components of coupled field scale reactive transport models.

Coupled transport and scaling are also highlighted in an upcoming NRC report on nonaqueous phase liquids (NAPLs) source zone assessment and remediation (NRC, 2004), and coupled reactive transport is an issue because biogeochemical processes result in a contaminant plume with a different composition than the original NAPL source. Coupled reactive transport models are also needed that describe the geochemical interactions and reactive transport behavior of contaminants such as U, 129I, and CCl4 in the varied geohydrochemical environments and sediment facies found at DOE sites such as in the Hanford vadose zone and unconfined aquifer. The influence of waste source composition, temperature, co-contaminants, and other properties on reaction chemistry (e.g. sorption, incorporation, precipitation) requires explicit consideration.

Thus the following research priorities and avenues of research are the focus of this Notice.

Contaminants

DOE sites across the United States contain over 6 billion cubic meters of contaminated soil, groundwater, and other environmental media (NRC, 2000a). Contaminants of concern across the DOE complex broadly include: radionuclides, metals, and nonaqueous phase liquids (NAPLs). Key contaminants (and their mixtures) of interest for this Notice are:

- Radionuclides: plutonium, strontium-90, cesium-137, technetium-99, iodine-129, neptunium-237, and uranium;
- Non-Radioactive Metals: chromium(VI) and mercury; and
- NAPLs: carbon tetrachloride, trichloroethylene, dichloroethylene, tetrachloroethylene, chloroform, dichloromethane, and polychlorinated biphenyls.

A description of the nature and extent of contamination at the principal DOE sites is available at http://www.nap.edu/books/0309065496/html/index.html/. More detailed information is available in some cases from the major DOE sites: Hanford (http://www.hanford.gov, http://www.hanford.gov/cp/gpp/, http://www.hanford.gov/cp/gpp/science/sandt.cfm)
Idaho National Laboratory (http://www.inel.gov/vadosezone/)
Oak Ridge Reservation (http://www.oro.doe.gov/em/) and
Savannah River Site (http://www.srs.gov/general/srs-home.html, http://www.srs.gov/general/enviro/erd/extpage.html)

Integrated Research Needs

This Notice has the primary objective of achieving scientific advances in our ability to better define and predict contaminant fate and transport in multidimensional heterogeneous (i.e., real world) systems.

Two principal scientific topics have emerged that cross-cut the program needs described above (NRC, 2001b, NRC, 2004, Anderson et al, 2004, Davis et al, 2004). First, contaminant or co-contaminant subsurface behavior results from a complex interplay of geologic, hydrologic, chemical, and biological processes and reactions. These processes are often coupled and interdependent, and a multidisciplinary approach must be used to incorporate these dependencies into conceptual modeling and into developing strategies for remediation, including containment and stabilization. Second, the processes occur over different spatial and temporal scales in the subsurface, often in heterogeneous media and flow regimes. Scaling methods must therefore address transitions in contaminant chemistry and water movement and changes in contaminant spatial distributions driven by system heterogeneities. These topics form the basis for this Notice. Research applications are solicited in the following areas:

- Coupled reactive transport: Observational, experimental and integrated computational approaches to examine the coupling of biological, chemical, mineralogical, and hydrogeologic processes controlling contaminant and co-contaminant transport.
- Nested or aggregated scale models: Experimental and computational approaches to extrapolate information across spatial scales with the ultimate goal of realistic process and parameter upscaling in subsurface systems.

Successful research in these areas requires close integration of observations of process coupling at different scales into better conceptual models. A desirable product of these studies would be the definition of constitutive relationships that would enable application of the research results to different locations in the DOE site complex. It is expected that successful approaches will entail strong interdisciplinary interactions and integrated experimental and computational components. For example, new methods and approaches, supported by laboratory and field measurements, are needed to describe and model the coupled microbial and chemical reactions that control contaminant behavior at the microscopic and pore-scales and to derive fundamental relationships that can be used in conjunction with scale-dependent physical properties to improve reactive transport modeling across larger spatial and time scales. An illustration of the types of processes and the range of scales considered pertinent to this Notice is given on page 135 of the SCaLeS (A Science-Based Case for Large Scale Simulation) program document (DOE, 2004) While

research has traditionally been targeted within each scale (see illustration at http://www.pnl.gov/scales/docs/SCaLeS_v2_draft_toc.pdf), methods to bridge between the scales is needed. Research may span all or part of this spectrum in the subsurface up to, and including the zone of groundwater/surface water interaction. Research focused on a single set of DOE site geohydrologic conditions is encouraged to facilitate quantitative descriptions of transitions between different spatial scales and domains. However, this does not preclude innovative approaches based on data from distributed sites. Examples of DOE sites representing a range of geohydrologic conditions are given in the websites listed above.

Technological Research Needs

The development and application of new tools for parameter measurement and characterization from the molecular/microscopic to field scales is encouraged when incorporated into research efforts addressing the two topic areas of coupled reactive transport and scaling listed above. Examples include new methods for measurement of biogeochemical processes at the pore scale; new methods for high resolution imaging and mapping of heterogeneity; innovative use of isotopic geochemistry and "designer" tracers to identify contaminant sources, preferential flow paths and regions of contaminant attenuation; and natural analogs to assess transport over extended length and time scales. New methods for remote sensing and for characterization and speciation of contaminants are sought. The development and validation of these tools for use in the subsurface environment is expected to markedly extend DOE's ability to characterize and monitor subsurface environments and address research needs in this area identified by the National Academy of Sciences (NRC, 2000a, NRC, 2000b, NRC, 2001a) and DOE (DOE, 2001a).

Availability of User Facilities and Other Specialized Resources

The ERSD within the DOE Office of Biological and Environmental Research (http://www.science.doe.gov/ober/ERSD_top.html) has responsibility for programs and facilities that offer unique and complementary resources for conduct of EMSP research. Potential applicants are encouraged to consider use of these programs/facilities in development of applications.

- The Field Research Center (FRC) at Oak Ridge National Laboratory (http://www.esd.ornl.gov/nabirfrc/index.html) provides a DOE site location where scientists can conduct field scale research and obtain DOE relevant samples of soils, sediments, and ground waters for laboratory research. A useful general orientation for prospective investigators is available at http://public.ornl.gov/nabirfrc/workshop2004_presentations.cfm.
- The Environmental Molecular Science Laboratory (EMSL) at the Pacific Northwest National Laboratory, (http://www.emsl.pnl.gov), is operated by ERSD as a national scientific user facility with state-of-the-art instrumentation in environmental spectroscopy, high field magnetic resonance, high performance mass spectroscopy, high resolution electron microscopy, x-ray diffraction, and high performance computing.
- The EMSL's high performance supercomputer is available for computational research in the physical, chemical and biological sciences, including molecular thermodynamics and

kinetics, heavy element chemistry, geochemistry, surface chemistry and groundwater flow and transport simulations (http://www.emsl.pnl.gov/capabs/mscf.shtml). Remote and on-site access to the 11+ TeraFlops, Linux-based Hewlett-Packard system and associated software, plus visualization and data storage capabilities is available through a separate application and external peer review process. Proposals for allocations of large blocks of time on the EMSL's HP system are solicited annually (usually in February or March for allocations beginning in October). Awards typically average 500,000 hours for multi-investigator teams (http://mscf.emsl.pnl.gov/about/allocation.shtml). DOE also provides compute cycles to the scientific user community at other high performance computing centers. For example, the National Energy Research Supercomputing Center (NERSC) at the Lawrence Berkeley National Laboratory provides a 10+ TeraFlops IBM system plus extensive data storage capabilities (http://www.nersc.gov). NERSC usually solicits proposals for time allocations in June or July. Proposals are externally peer reviewed and time awards are announced in December. The Center for Computational Science (CCS) at the Oak Ridge National Laboratory has several supercomputers available to users, including a Cray X-1, two IBM-based systems, and an SGI Altix system (http://www.ccs.ornl.gov). Proposals for time allocations on the various systems at the CCS may be submitted throughout the year, but will be subject to an internal peer review process (http://www.ccs.ornl.gov/accounts/acct-FAQ.html).

- ERSD (http://www.sc.doe.gov/ober/ober_top.html) provides user support for experiments at synchrotron light sources that are capable of providing structural and chemical information often unavailable with conventional sources of x-rays. DOE laboratories with synchrotrons supporting ERSD research and points of contact include: Argonne National Laboratory (http://www.aps.anl.gov/index.html), contact Ken Kemner (kemner@anl.gov); Brookhaven National Laboratory (http://www.nsls.bnl.gov/), contact Jeffrey Fitts (fitts@bnl.gov); Lawrence Berkeley National Laboratory (http://esd.lbl.gov/als_environmental_program/), contact Susan Hubbard (sshubbard@lbl.gov); and Stanford Synchrotron Radiation Laboratory (http://www-ssrl.slac.stanford.edu/mes/remedi/index.html), contact John Bargar, bargar@slac.stanford.edu). Use of the synchrotron light sources requires a separate approval process.

Merit Review

Applications will be subjected to formal merit review (peer review) and will be evaluated against the following evaluation criteria which are listed in descending order of importance codified at 10 CFR 605.10(d):

1. Scientific and/or Technical Merit of the Project;
2. Appropriateness of the Proposed Method or Approach;
3. Competency of Applicant's personnel and Adequacy of Proposed Resources;
4. Reasonableness and Appropriateness of the Proposed Budget.

For renewals, progress on previous ERSD funded research will be an important criterion for evaluation. As part of the evaluation, program policy factors also become a selection priority. Note, external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Federal and non-federal reviewers will be used, and

submission of an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

Submission Information

Information about the development, submission of applications, eligibility, limitations, evaluation, the selection process, and other policies and procedures may be found in 10 CFR Part 605, and in the Application Guide for the Office of Science Financial Assistance Program. Electronic access to SC's Financial Assistance Application Guide is possible via the World Wide Web at: http://www.science.doe.gov/grants/. DOE is under no obligation to pay for any costs associated with the preparation or submission of applications.

In addition, for this notice, the research description must be 20 pages or less, exclusive of attachments, and must contain an abstract or summary of the proposed research (to include the hypotheses being tested, the proposed experimental design, and the names of all investigators and their affiliations). **Applicants who have current ERSD support (i.e., renewal applications) must include a Progress Section with a description of results, the funding history (i.e., number of years and amounts per year for all PI's and co-PI's), and a list of publications derived from that funding.** Attachments should include short (2 pages) curriculum vitae, QA/QC plan, a listing of all current and pending federal support and letters of intent for proposed collaborators (when applicable). Curriculum vitae should be submitted in a form similar to that of NIH or NSF.

Grantees must comply with federal and state laws and regulations as appropriate; for example, the Toxic Substances Control Act (TSCA) as it applies to genetically modified organisms. Although compliance with NEPA is the responsibility of DOE, grantees proposing to conduct field research are expected to provide information necessary for the DOE to complete the NEPA review and documentation.

Information about ERSD programs on the role of microbes in contaminant remediation and transport can be found at: http://www.lbl.gov/NABIR/. The ERSD may issue further Notices on the role of microorganisms on contaminant metals and radionuclides during FY 2005. Applications focused on the use of biological processes for *in situ* remediation should respond to these other Notices. Applications featuring biological affects on coupled reactions and on upscaling issues in contaminant fate and transport should be submitted to this Notice.

REFERENCES

Note: World Wide Web locations of these documents are provided where possible. For those without access to the World Wide Web, hard copies of these references may be obtained by contacting Roland Hirsch at the electronic mail address listed in the FOR FURTHER INFORMATION CONTACT section.

Anderson, S.P.; J. Blum; S.L. Brantley; O. Chadwick; J. Chorover; L.A. Derry; J.I. Drever; J.G. Herring; J. W. Kirchner; L.R. Kump; D. Richter; A.E. White 2004. Proposed Initiative Would Study Earth's Weathering Engine EOS 85, 265-269.

Davis, J.A.; S.B. Yabusaki; C.I. Steefel; J.M. Zachara; G.P. Curtis; G.D. Redden; L.J. Criscenti; B.D. Honeyman 2004. Assessing Conceptual Models for Subsurface Reactive Transport of Inorganic Contaminants EOS 85, 449-455.

Department of Energy, 2001a. A National Roadmap for the Vadose Zone Science & Technology. http://www.inel.gov/vadosezone/

Department of Energy, 2001b. A Report to Congress on Long-Term Stewardship. Office of Environmental Management. Washington, DC.

Department of Energy, 2004. A Science-Based Case for Large Scale Simulation. Vol. II. Office of Science, United States Department of Energy. Washington, DC http://www.pnl.gov/scales/docs/SCaLeS_v2_draft_toc.pdf

National Research Council, 2000a. Research Needs in Subsurface Science, U.S. Department of Energy's Environmental Management Science Program. National Academy Press, Washington, DC. http://www.nap.edu/browse.html

National Research Council, 2000b. Seeing into the Earth: Noninvasive Characterization of the Shallow Subsurface for Environment and Engineering Application, U.S. Department of Energy's Environmental Management Science Program. National Academy Press, Washington, DC. http://www.nap.edu/browse.html

National Research Council, 2001a. A Strategic Vision for Department of Energy Quality of Research and Development. National Academy Press, Washington, DC. http://www.nap.edu/browse.html

National Research Council, 2001b. Science and Technology for Environmental Cleanup at Hanford. National Academy Press, Washington, DC. http://www.nap.edu/browse.html

The Catalog of Federal Domestic Assistance number for this program is 81.049, and the solicitation control number is ERFAP 10 CFR Part 605.

Martin Rubinstein
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Posted on the Office of Science Grants and Contracts Web Site
December 27, 2004.