U.S. Department of Energy
Office of Science

Office of Biological and Environmental Research
Environmental Remediation Sciences Division

ENVIRONMENTAL REMEDIATION SCIENCES PROGRAM STRATEGIC PLAN

Providing the scientific basis to solve DOE's intractable problems in environmental remediation and long-term stewardship"

September 2007

Foreword

The Environmental Remediation Sciences Division (ERSD) resides within the Office of Biological and Environmental Research (BER), one of six program offices within the U.S. Department of Energy's (DOE's) Office of Science (SC). ERSD supports two major activities: a scientific research program, the Environmental Remediation Science Program (ERSP), that seeks to provide the fundamental scientific knowledge needed to address challenging environmental problems that impede the remediation of contaminated environmental sites; and the W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL), a national scientific user facility located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington, which provides integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences. This Strategic Plan focuses on the research program—ERSP—and is written in the context of the DOE-SC Strategic Plan. The EMSL Strategic Plan can be found at http://www.emsl.pnl.gov/.

DOE is responsible for what has been described as the largest, most complex, and diverse collection of environmental remediation challenges in the nation. While some of the problems are tractable and require only time and money to resolve, a large fraction of them cannot be resolved with existing knowledge and technology. It is the need for solutions to this subset of environmental remediation problems that drives the ERSD research program. Progress toward this long-term goal is evaluated by quarterly, annual, and long-term measures.

The Administration has established a formal process for developing and evaluating program performance: the Program Assessment Rating Tool (PART). The PARTs are diagnostic tools that rely on professional judgment to assess and evaluate programs across a wide range of issues related to performance. BER supports four long-term PART measures, including the one adopted by ERSD in 2005 (and modified in 2006) that by 2015, the Division will "provide sufficient scientific understanding such that DOE sites would be able to incorporate coupled physical, chemical and biological processes into decision making for environmental remediation and long-term stewardship." This Strategic Plan outlines the approach that ERSD will take to fulfill that measure.

The long-term measure recognizes the importance of natural processes and their interactions at different scales in controlling the fate and transport of DOE contaminants in the subsurface. The measure also recognizes that DOE's remediation challenges occur in the field and that our understanding of contaminant behavior must be broadly applicable to individual DOE sites. ERSD will continue to encourage field or field-relevant research designed to provide critical understanding in support of decision making across the DOE complex.

This Strategic Plan recognizes a suite of DOE-relevant contaminants including radionuclides, other toxic metals, and organic contaminants. While funding has historically limited the breadth of research in ERSD to primarily inorganic contaminants, the importance of all of these chemical families to the DOE cleanup challenge is recognized, and efforts will continue to expand the breadth of research to include all relevant contaminants.

ERSD supports externally peer-reviewed research in collaborative fundamental science using interdisciplinary approaches to address environmental remediation and stewardship of DOE sites. ERSD supports the activities of the DOE Offices of Environmental Management, Legacy Management, and Civilian Radioactive Waste Management through close and active collaboration.

ERSD is committed to seeking input from the scientific community and providing consistent and transparent management supporting the overall scientific community and advancing DOE's mission in environmental remediation. While scientific findings, DOE priorities, and funding levels change over time and will alter the specific content of program solicitations, this Strategic Plan encompasses the major DOE environmental remediation challenges that can benefit from long-term, basic scientific research.

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Contents

1.0 Introduction

The U.S. Department of Energy (DOE) is faced with a daunting legacy of the Cold War: the environmental management of the nuclear weapons complex consisting of more than 5000 surplus facilities and associated land located at 144 sites in 31 states and a U.S. territory (DOE 1997, 1999). More than 380,000 cubic meters of high-level radioactive waste is estimated to be stored at several sites, and the total volume of soil, groundwater, and sediment present in highly diverse environments and contaminated with complex mixtures of radionuclides, metals, and organic contaminants may exceed 1800 million cubic meters (DOE 1997, 1999; Crowley and Ahearne 2002). Waste treatment, environmental remediation, and long-term stewardship of these sites are estimated to require hundreds of billions of dollars and major breakthroughs in science and technology to accomplish.

DOE's Office of Biological and Environmental Research (BER) has a long tradition of supporting fundamental research to address DOE's intractable problems. Research has been under way in this office for nearly two decades to understand and harness natural processes for remediating environments contaminated as a result of the production of nuclear weapons and materials and associated disposal practices.

BER's Environmental Remediation Sciences Division (ERSD) supports the major DOE scientific programs involved in remediation research as well as the W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL) located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. ERSD has made remarkable progress in developing new waste treatment, separation, and stabilization concepts and in understanding the physical, chemical, and biological processes that interact at multiple scales to control contaminant form and transport in the environment. However, new paradigms are needed for addressing the most challenging waste treatment and environmental contamination issues that remain as a legacy of nuclear-defense programs at DOE sites.

New knowledge and tools are rapidly evolving from DOE Office of Science (SC) initiatives to address important gaps in our understanding of the molecular sciences, fathom the machinery of life, and develop the computational power and infrastructure to simulate and scale complex interdependent phenomena, and these advances are setting the stage for an exciting new era in remediation sciences. ERSD was restructured in FY 2006 to take full advantage of these resources and help provide the scientific foundation for environmental remediation and stewardship of DOE sites. Figure 1 illustrates ERSD's multidisciplinary investigations in four key areas that are integrated through research at field sites, from the molecular to field scales.

The purpose of this document is to communicate to a broad audience the strategy with which ERSD plans to implement its mission. This strategy was developed in concert with recommendations from the Biological and Environmental Research Advisory Committee (BERAC) assessment process and the scientific and user communities. The success of the strategy will depend on the creativity and resourcefulness of the scientific and user communities and their collaboration in applying the research results to achieve DOE's environmental remediation and stewardship goals. ERSD is committed to implementation of a strong fundamental scientific program implemented in concert with, and addressing the needs of the DOE sites.

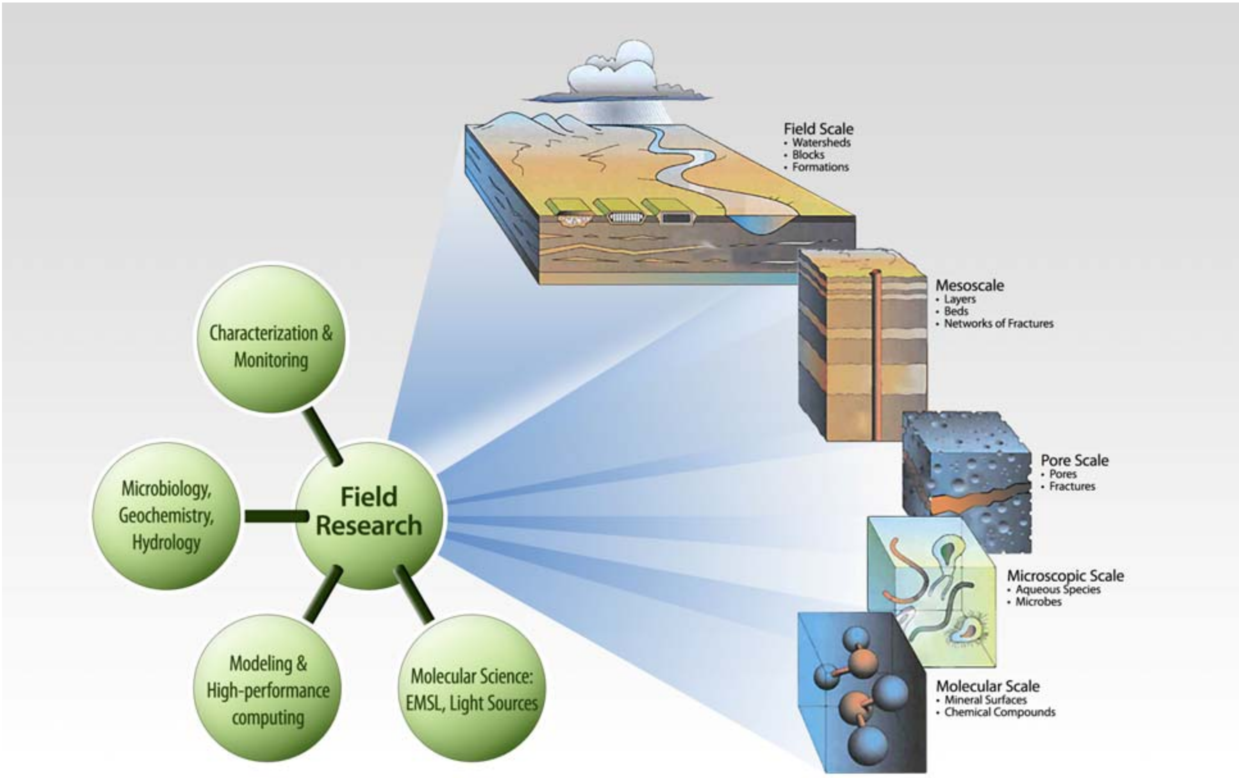


Figure 1. DOE's remediation challenges occur in the field where highly interactive natural processes occur over a broad range of scales control the fate and transport of contaminants. The ERSD goal is to help provide the basis for development of innovative remediation measures and to support decision making critical to long-term site stewardship.

2.0 Mission

The mission of the ERSD is

To advance our understanding of the fundamental biological, chemical, and physical processes that control contaminant behavior in the environment in ways that help solve DOE's intractable problems in environmental remediation and stewardship.

The fundamental nature of the research supported by ERSD will ensure that the results will be broadly applicable to other DOE missions.

The ERSD mission is accomplished through hypothesis-driven, discovery-based fundamental research. Research is implemented through competitively awarded, peer-reviewed research projects at scientific institutions nationwide and through a network of DOE-SC research programs and scientific user facilities and research sites that provide unique capabilities to probe and understand the physical, chemical, and biological nature of our environment.

ERSD research will build on the knowledge base and capabilities developed by the world-wide scientific community, including more than 50 years of BER research to assess the environmental effects of our nation's nuclear-defense program. Examples of DOE capabilities (detailed in Section 5) include

- The EMSL, a national scientific user facility sponsored by ERSD and located at PNNL in Richland, Washington, that provides expertise, leading-edge instrumentation, and high-performance computational capabilities for molecular-level environmental research
- Three field sites supported to conduct multidisciplinary field scale research. Two of these field sites (Oak Ridge, Tennessee and Old Rifle, Colorado) represent a new format for directed research that continues ongoing subsurface science at these sites. The third site provides a framework for a more focused, integrated research effort at the Hanford 300 Area (Washington State). These sites are an important component of ERSP-funded research enabling the testing of laboratory-derived hypotheses under natural conditions at the field scale as well as the acquisition of real world samples from contaminated and uncontaminated environments.

ERSD also provides user support for the synchrotron light sources that are available through collaboration with the DOE Office of Basic Energy Sciences (BES), and collaborates closely with other unique programs such as the BER Genomics: GTL program, the DOE Office of Advanced Scientific Computing Research (ASCR), and the Environmental Molecular Science Institutes (EMSIs), jointly supported with the National Science Foundation (NSF). ERSD encourages integration of rapidly developing new capabilities and tools in the biological, chemical, physical, and computational sciences to advance our understanding of natural environments, devise remediation strategies, and ensure the success of long-term stewardship in support of the overall DOE mission.

3.0 Long-Term Performance Measure

As part of the strategic planning process, a long-term measure of ERSD performance has been established that will be used in the Federal Program Assessment Rating Tool (PART) process to establish consistent performance ratings and guide budget decisions (http://www.sc.doe.gov/measures/). The PART was developed by the Office of Budget and Management in collaboration with other Federal agencies. It establishes a high, "good government" standard of performance and will be used to rate programs in an open, public fashion. Ratings for 20% of programs will be published in the FY 2004 Budget, and the basis for the rating made available to the public.

3.1 Measure of Success

The long-term measure of ERSD success is as follows:

By 2015, provide sufficient scientific understanding such that DOE sites would be able to incorporate coupled physical, chemical and biological processes into decision making for environmental remediation and long-term stewardship.

3.1.1 Why This Measure is Important

The DOE complex presents, arguably, the most daunting subsurface environmental remediation and stewardship challenges facing the nation. Of the 144 sites where DOE has remediation, waste management, or nuclear material and facility stabilization responsibilities, more than 100 have soils, sediments, or groundwater contaminated with radionuclides, metals, or organic materials. These sites represent a broad range in climatic, ecologic, and geohydrologic conditions and are expected to require long-term stewardship (DOE 1999, 2001). Today's remediation technologies—primarily soil excavation and disposal and long-term pumping and treating of groundwater—are limited in their application and effectiveness and can be cost prohibitive. Sites for which active remediation has been completed often contain residual contamination that must be managed and monitored over the long term to protect human health and the environment.

Long-term stewardship of these sites, under the jurisdiction of the DOE Office of Legacy Management (LM) (http://www.lm.doe.gov/) will require innovative concepts and tools to assess the effects of natural attenuation processes and monitor the long-term behavior of contaminants (DOE 1999). Decisions to predict the probability of success of and implement closure measures—ranging from no-action alternatives and site stewardship to complete excavation and off-site disposal—need to be based on a sound scientific understanding of the complex subsurface environments and processes controlling contaminant fate and transport. Furthermore, a fundamental knowledge of these processes can be used to devise novel approaches to remediation, ranging from direct *in situ* manipulation of biogeochemical and/or physical processes to monitored natural attenuation and long-term stewardship.

3.1.2 What is Needed to Meet This Measure

Understanding and predicting contaminant fate and transport and developing new, cost-effective concepts for subsurface remediation will depend on a robust understanding of biological, chemical, and physical processes and their interactions that collectively control contaminant fate and transport in the broad range of geologic and climatic regimes throughout the DOE complex. This will require fundamental advances in our understanding of the constitutive relationships governing water and contaminant transport over the long term and the development of conceptual and numerical models that span the multiple spatial and temporal scales typical of subsurface hydrogeologic environments.

The results will be advanced understanding of the critical processes that determine contaminant fate and transport in the subsurface; improved, scientifically credible predictions of water and contaminant transport; and new remediation concepts based on fundamental understanding of subsurface processes. This will in turn lead to advances in the ability of site personnel to make critical decisions on the need for remediation as well as the nature, location, extent, and timing of remedial actions and monitoring.

3.2 ERSD's Goals and Research Program

The overarching goals established to meet the requirements of DOE, as expressed in the ERSD Performance Measure, and to address key issues in environmental remediation and site stewardship are given in Table 1 along with expected accomplishments over the next decade. The ERSD goals build on those described in the previous ERSD Strategic Plan (DOE 2004a) and reflect intervening research accomplishments and changes in the scope of ERSD responsibilities. The scope, background and rationale, and research priorities for each of the principal ERSD goals are given below.

3.3 Goal 1 – Understand and Predict Contaminant Fate and Transport

Develop an improved understanding of the processes governing the fate and transport of contaminants to predict and control the long-term performance of environmental remediation and facilitate stewardship of DOE sites.

3.3.1 Scope

Research will be directed toward establishing the constitutive relationships governing the coupling and scaling of biological, geochemical, and physical processes in heterogeneous field environments. Emphasis will be on development of conceptual and numerical models that represent the key processes controlling contaminant form and mobility in representative DOE environments. This knowledge will be used to construct numerical simulations of contaminant mobility at the levels of complexity and scale and over the time periods needed for long-term stewardship of DOE sites. Predictive models can then serve as the basis for decision-making as well as selection and design of remediation methods and monitoring strategies.

Table 1. Scientific goals and expected accomplishments

Division Goal (Scientific focus)	**Near-Term Priorities (<6 years)**	**Intermediate-Term Priorities (3-9 years)**	**Long-Term Priorities/Results (>9 years)**
1. Develop an improved understanding of the processes governing the fate and transport of contaminants to predict and control environmental remediation and facilitate stewardship of DOE sites (*constitutive relationships governing the coupling and scaling of natural processes in heterogeneous field environments*)	Integrated experimental approaches to describe coupling of biological, chemical and hydrogeologic processes at different (field-relevant) spatial scales Development of coupled conceptual/numerical models for realistic process and parameter upscaling in representative field environments	New approaches to assess spatial and temporal changes in water and contaminant transport for long-term stewardship. Incorporation of high-performance computational tools into predictive models, linking multiple processes at different spatial and temporal scales Experimental verification of coupled fate and transport models through long-term field studies.	Large-scale, fully coupled transport simulators.
2. Explore new options and concepts for remediation of subsurface systems (*biologically mediated and hydrogeochemical phenomena influencing the form and mobility of DOE contaminants and remediation strategies*)	Build on new tools in genomics and proteomics developed in the Genomics: GTL program to explore the genetic diversity and dynamics of microbial communities Define and exploit microbial metabolic processes critical to controlling contaminant mobility Determine key redox/complexation reactions and degradation pathways involved in radionuclide/metal and organic transformations and immobilization Use and advance tools and techniques in microscopy and spectroscopy to determine the form and stability of immobilized contaminants over the long term.	Gene regulation and expression for salient contaminant transformation processes in natural systems Long-term biogeochemical reaction kinetics and the integrated response to manipulation of or natural change in environmental conditions.	Sound foundation for remedial action decisions and development of novel *in situ* remediation strategies

Table 1. (Contd.)

Division Goal (Scientific focus)	**Near-Term Priorities (<6 years)**	**Intermediate-Term Priorities (3-9 years)**	**Long-Term Priorities/Results (>9 years)**
3. Develop new measurement and monitoring tools to better understand and manage contaminant transport (*new approaches for interrogating biological, chemical and physical processes in natural environments*)	Innovative methods for rapid assessment of changes in microbial community composition and metabolic potential High-resolution, integrated geophysical methods for measuring biogeochemical and hydrologic responses to *in situ* manipulation of subsurface systems Fundamental tools for assessing chemical speciation in sediments and waters Geophysical and chemical sensing tools that target key physical/chemical features controlling gaseous and fluid movement in unsaturated and saturated environments	Integrated sensor, isotopic, and natural analog concepts and approaches for evaluating system response and change Refine monitoring packages to include wireless, miniaturization, and visualization technologies. Incorporate and test new tools and approaches in field studies (Goals 1, 2)	Field-validated, robust tools for validation of predictive models and remediation strategies and for long-term performance monitoring

3.3.2 Challenges

One of the most vexing scientific problems facing DOE has been how to characterize, predict, and control subsurface contaminant migration at DOE sites. This information will be critical to assess risk, determine the need for remediation, and—where needed—develop, apply, and evaluate innovative remediation methods to contain, attenuate, transform, or remove contaminants. The need to predict and control contaminant mobility over the long term is reinforced by DOE estimates that more than 100 sites will have residual contamination once cleanup programs are completed (DOE 1999).

Key needs in DOE long-term site stewardship that were identified by the National Research Council (NRC 2000a, 2003) include simulating and predicting the fate and transport of contaminants in multidimensional heterogeneous (i.e., real-world) systems, developing appropriate remediation or stabilization methods based on this knowledge, and assessing the performance of both predictive models and mitigation efforts over the long term.

The inherent complexity of the subsurface and our limited ability to observe processes and interactions as they occur in these systems have proven to be major obstacles 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 2004b) called for interdisciplinary laboratory and field investigations of subsurface processes at all fundamental length scales.

The inherent complexity of the subsurface and our limited ability to observe processes and interactions as they occur in these systems have proven to be major obstacles to predictive simulation of contaminant behavior at the field scale.

3.3.3 Research Priorities

Two principal crosscutting scientific needs have emerged from assessments of research needs in contaminant fate and transport (NRC 2001b; Anderson et al. 2004; Davis et al. 2004), and these form the basis for ERSD research in this area. 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 require a multidisciplinary approach to incorporate these dependencies into conceptual models and to develop remediation strategies. Second, the processes occur over different spatial and temporal scales in the subsurface, often in complex and changing 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 science needs are supported by the following research priorities:

- Build on a field-oriented, integrated research program to understand the constitutive relationships governing the coupling of biological, geochemical, and hydrogeologic process at field-relevant temporal and spatial scales.
- Develop new approaches for measurement of key physical and geochemical features controlling fluid and solute movement in heterogeneous systems (see Goal 3).
- Refine and test integrated sensor, isotopic, and natural analog concepts for evaluating subsurface system-level response to changes in biological, geochemical, and flow characteristics. Site

ERSD research has demonstrated the profound influence that alterations in subsurface microbiology and geochemistry can have on contaminant behavior and the importance of understanding these processes in the context of site hydrogeology.

stewardship requires the ability to measure changes in these properties over long time frames (see Goal 3).

- Develop and validate predictive transport and remediation models using high-performance computational tools to incorporate long-term biogeochemical reaction kinetics and fluid dynamics and to link multiple processes at different spatial and temporal scales.
- Experimentally verify coupled fate and transport models through integrated laboratory, intermediate-scale and long-term field studies.

Principal accomplishments expected from research to address Goal 1 over the next decade are outlined in Table 1.

3.4 Goal 2 – Subsurface Remediation and Long-Term Stewardship

Explore new options and concepts for remediation and long-term stewardship of subsurface systems.

3.4.1 Scope

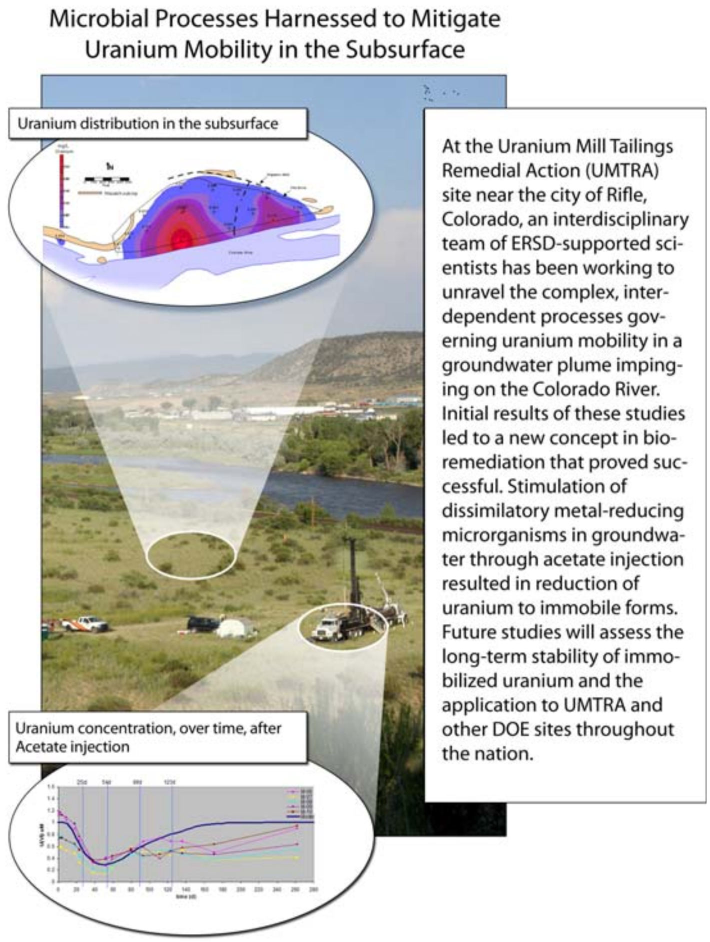
The ERSD will build on fundamental knowledge of naturally, hydrogeochemically, and biologically mediated phenomena to provide new concepts and strategies for effective remediation and long-term stewardship of DOE sites. DOE's remediation problems are field problems, and research will increasingly be directed toward field environments to ensure relevance of the research to real needs, building on the results of research described in Goal 1. Research will be directed toward situations where few, if any, cost-efficient remediation technologies exist; that is, subsurface systems at DOE sites with low or intermediate levels of contamination below the zone of root influence. To the extent possible, Goal 2 will be done in parallel with Goal 1.

The remediation program will emphasize contaminants that are unique to DOE and comprise a significant fraction of the DOE waste inventory, are potentially mobile and dispersed in the subsurface under certain conditions, and drive human and/or environmental risk estimates at DOE sites. These include radioactive elements, other toxic metals, organic compounds that may influence the behavior of DOE-relevant radionuclides and metals (e.g., co-disposed complexing agents), and non-aqueous phase liquids (NAPLs) and their partition/degradation products. Emphasis will be placed on understanding the subsurface features and processes that govern the form and mobility of these contaminants with the goal of predicting (Goal 1) and controlling (Goal 2) their behavior. Initial remediation concepts to be explored will be based on subsurface biological, chemical, and physical processes, which singularly or in combination have the potential for contaminant *in situ* immobilization, transformation, or degradation.

3.4.2 Challenges

ERSD research has helped to create a fundamental understanding of subsurface microbiology, geochemistry, and hydrogeology that is serving as a basis for new remediation concepts based on natural phenomena.

Research in the ERSD Natural and Accelerated Bioremediation Research (NABIR) program has demonstrated the profound influence that alterations in subsurface microbiology and geochemistry can have on contaminant behavior and the importance of understanding these processes in the context of site hydrogeology. Biologically driven manipulation of the redox state of sediment mineral surfaces and contaminants in the field now appears feasible and has strong potential for limiting the transport of soluble metals and radionuclides by altering their oxidation state. Bioprocesses may also enhance the degradation of organic compounds such as the chlorinated hydrocarbons in contaminated groundwater aquifers. For example, the transport of contaminants that form highly mobile oxyanions, such as uranium, chromium, and technetium, has been shown to be markedly altered by addition of suitable electron donors (DOE 2006).



ERSD fundamental research in cooperation with the DOE Office of Legacy Management has led to new concepts for use of subsurface processes to immobilize contaminants in the subsurface. Current field research efforts at the NABIR Integrated Field Research Challenge located on the Oak Ridge Reservation, at Uranium Mill Tailings Remedial Action (UMTRA) sites, and at the Hanford site are taking the first major steps toward documenting, modeling, and attempting to control *in situ* microbial processes affecting metal and radionuclide transport at the field scale. Yet, science has just begun to explore the diversity of subsurface microbial communities and microbial community structure and metabolism as a function of (natural or induced) environmental conditions, as well as the potential role of microbially catalyzed biogeochemical processes in contaminant transformations.

New capabilities and mathematical descriptions are needed to quantitatively relate microbial growth and activity to contaminant transformations and to incorporate this information into reactive transport codes (Goal 1). Advanced molecular-based tools and capabilities arising from the Genomics: GTL program (http://genomicsgtl.energy.gov/) will be needed to assess microbial diversity and function and to interrogate cellular and subcellular processes. Genome-enabled technologies will need to be linked with high-resolution microscopies, spatially specific spectroscopies, and advanced imaging methods to probe cell-mineral attachment mechanisms, electron and chemical dynamics at the cell-mineral interface, and the formation of new mineralogical phases. These are important processes in the control of contaminant transformation kinetics and the long-term stability of immobilized transformation products.

The broad range of contamination problems faced by DOE at different sites will require consideration of the full spectrum of potential *in situ* remediation technologies. In addition to biologically based subsurface processes, ERSD will build on the results of past research in subsurface systems to develop novel remediation concepts based on fundamental knowledge of physical and geochemical properties and processes. Research will be directed toward determining how these processes might be used selectively and in combination to mitigate the mobility of inorganic contaminants and degrade organic contaminants at sites representing the diverse environmental conditions present on the DOE complex and for the long time periods that must be addressed in stewardship of DOE sites.

3.4.3 Research Priorities

Future research will be intricately tied to research now under way in the ERSD to develop conceptual models describing the coupling and scaling of subsurface processes controlling contaminant transport. It will demonstrate how these processes control the composition and metabolic potential of subsurface microbial communities and establish the basis for new field-based remediation concepts that take advantage of natural hydrogeologic features or stimulated microbial and geochemical processes for remediation of subsurface environments. Overall research priorities are to

- Apply advances in microbial genetics and proteomics from Genomics: GTL research to explore the genetic diversity and dynamics of microbial subsurface communities and develop novel *in situ* remediation concepts for altering contaminant form and mobility, and assess the impact of remediation on natural systems.
- Determine the dominant electron donors/acceptors fueling microbial metabolic processes under reducing conditions and the dominant pathways for radionuclide/metal and organic transformations and sequestration.
- Explore new field-based remediation/attenuation concepts based on fundamental knowledge of subsurface hydrogeologic and geochemical properties and processes.
- Build conceptual models describing the integrated response of subsurface systems to predict and subsequently manipulate environmental conditions (such as nutrient availability, electron donors/acceptors, pH) and the form and stability of contaminant degradation and sequestration products over the long term.

Principal accomplishments expected from research to address Goal 2 over the next decade are outlined in Table 1.

3.5 Goal 3 – New Measurement and Monitoring Approaches

Provide the scientific foundation for new measurement and monitoring tools to better understand and manage contaminant transport.

3.5.1 Scope

A major challenge is to develop the next generation of coupled measurement and numerical approaches that optimize the use of non-invasive geophysical tools while providing the hydrologic and geochemical information at scales necessary for assessing contaminant behavior.

Research in ERSD provides the fundamental scientific basis for developing new concepts and integrated measurement and numerical approaches for locating contamination in the near field (immediate vicinity of tank waste leaks where the contamination may be present in concentrations sufficient to alter the environment) and far field (where natural processes become more influential than waste components) and for determining contaminant and subsurface properties critical to predicting contaminant long-term behavior. New approaches will be developed to visualize the relevant features and properties of the subsurface in three dimensions and couple remote geophysical methods of lower resolution with point measurements of biological, contaminant, and geochemical phenomena to better represent the processes controlling contaminant form as well as spatial and temporal distributions in the subsurface.

3.5.2 Challenges

New concepts and tools are needed for locating and assessing the concentration and chemical speciation of contaminants in the subsurface, and for understanding the physical, chemical, and biological processes that control contaminant behavior in the heterogeneous, highly diverse climatological and geohydrologic regimes represented in the DOE site complex (NRC 2000a, 2001a). At many sites, the nature and extent of subsurface contamination is poorly known, and available methods for detection do not adequately meet site needs in assessment of risk or in design, implementation and long-term monitoring of remedial actions.

There is a general lack in the ability to adequately describe heterogeneity in physical, chemical, and biological properties at multiple scales and to temporally and spatially define biochemical reactions related to water flow. In fact, the full extent of variability is not understood in most environments. As the ability to resolve key features and processes in controlled environments evolves (NRC 2000b), so does the appreciation of the potential importance of variability at smaller scales (e.g., “microenvironments”).

Direct methods for subsurface characterization (i.e., sampling from boreholes), are expensive, limited in range to the core segment examined, may inherently alter results, and can potentially exacerbate existing problems by creating pathways for wider dispersal of contaminants. Currently, geophysical measurements (e.g., seismic reflection, ground penetrating radar) offer the best and least-costly avenue for remote measurements of geologic/sedimentary features. However, these methods do not yet provide direct information on hydrologic parameters such as permeability or water potential or on chemical and biogeochemical parameters critical to locating contamination and predicting contaminant concentration, form, and mobility. Thus, a major challenge is to develop the next generation of integrated measurement and numerical modeling approaches that optimize the use of non-invasive geophysical tools while providing the hydrologic and geochemical information at scales necessary for assessing contaminant behavior.

3.5.3 Research Priorities

Current ground-based and cross-borehole geophysical methods will be refined and augmented with new *in situ* geochemical and microbiological measurements to better define water flow patterns, pore fluid composition, microbial community composition and metabolic response, and processes essential for prediction of contaminant form and distribution (e.g., kinetic controls on biogeochemical processes). A fundamental goal is to ensure that the necessary measurement and monitoring tools are available to support remediation performance assessment and site stewardship. Overall research priorities are to

- Reduce current constraints on conceptual model development by improving the range, specificity, and resolution of non-invasive, ground-based geophysical mapping tools (e.g., cross-borehole methods). Emphasis will be placed on basic research to remotely define subsurface physical properties (e.g., sediment lithologies) at scales that more closely correlate with chemical and biological properties important in defining contaminant reactive transport. When interpreted within the fabric of geophysical measurements, this knowledge will also markedly improve design and interpretation of site-specific sampling and sensor networks.
- Provide the fundamental basis for improved real time, remote or minimally invasive techniques for locating and determining the chemical speciation of contaminants *in situ* and the biological, physical and chemical properties of the environments in which the contaminants reside. Interdisciplinary research will be directed toward development of a new generation of *in situ* analytical approaches that build on advances in fundamental biology, chemistry, physics, nanoscience, photonics, fluidics, electronics, and miniaturization to provide new insights into subsurface properties through systems that are delivered down-hole.
- Develop and field-test sensor, isotopic, and natural analog approaches for evaluating subsurface system response and change. Fundamental research will be directed toward development of integrated measurement and numerical modeling tools (e.g., geophysical/geochemical measurements with process-based geologic models). Priority will be given to spatial and temporal resolution, and to interpolation and upscaling of subsurface properties and processes important to field validation of predictive models and remediation strategies.
- Develop minimally invasive high-resolution geophysical methods (e.g., integrated seismic, radar, and frequency-dependent electrical measurements) to characterize coupled processes (e.g., biologically mediated mineral precipitation and dissolution) occurring during *in situ* chemical manipulation and biological stimulation.

Principal accomplishments expected from research to address Goal 3 over the next decade are outlined in Table 1.

4.0 Program Integration and Management

The management and integration of this program need to be cognizant of and consistent with the nature, magnitude, and diversity of contamination problems at DOE sites nationwide. Successfully addressing the multiplicity of interactive biological, chemical, and physical processes that occur at different DOE sites and that govern contaminant behavior and remediation strategies requires a fully integrated, interdisciplinary research approach from the molecular to field scale. The imagination and expertise to develop new concepts for addressing these problems resides in scientific institutions throughout the United States and around the world, and ERSD has the responsibility for reaching out to the scientific community, fostering new approaches for resolution of some of the most difficult environmental contamination problems ever faced, and implementing and managing national programs that take full advantage of available resources.

The ERSD research portfolio is directed toward achieving the Overall Performance Measure (Section 3) and is centered on the three general goals and the research priorities described in this document and outlined in Table 1. Management and implementation of the research will be guided by the following commitments:

- ERSD staff committed to seeking input from the scientific community and providing current information on future plans.
- Management of ERSD in a predictable and transparent manner to support the overall scientific community and advance the DOE mission in environmental remediation.
- Externally peer-reviewed research in collaborative fundamental science (http://www.science.doe.gov/grants/Colab.html) and support of the interdisciplinary approaches critical to addressing environmental remediation and stewardship of DOE sites.
- Integration of existing research programs into a cohesive, fundamental remediation science program that can be managed to fully use available scientific resources, achieve realistic scientific objectives, and respond to new scientific discoveries and evolving DOE needs.
- Field-relevant research, taking maximum advantage of the ERSD IFCs as well as opportunities at other sites for controlled field studies and incorporation of fundamental research into environmental remediation programs.
- Close and active cooperation with the DOE Offices of Environmental Management (EM); Legacy Management (LM); and Civilian Radioactive Waste Management (RW).
- Enhanced synergies with other DOE programs (e.g., BER-Genomics: GTL, BES-Geosciences, and SciDAC) and other federal agencies (e.g., NSF, EPA), expanding the tools and expertise needed to support ERSD goals.
- Maximum leveraging of DOE user facilities (e.g., EMSL, light sources) to provide the advanced experimental and computational tools needed to address complex problems in environmental remediation.
- Permanent and temporary ERSD staff representing the range of scientific disciplines and interdisciplinary expertise needed for effective management and integration of the research programs.

- Research programs refreshed with annual research solicitations centered on consistent technical themes and information gaps and that address fundamental questions resulting from on-going research.
- A strong systematic technical approach and a supporting management structure will be necessary to ensure program integration and synergy.

5.0 Availability of User Facilities and Other Specialized Resources

The ERSD has responsibility for programs and facilities that offer unique and complementary resources for implementation of environmental remediation research. These resources include:

- The EMSL at PNNL, which is supported 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.
- ERSD funds three multidisciplinary field scale research program at three different field sites. These Integrated Field-Scale Subsurface Research Challenges (IFCs) are located at Oak Ridge, Tennessee; Old Rifle, Colorado; and the Hanford 300 Area (Washington State). These IFCs are an important component of ERSP-funded research enabling the testing of laboratory-derived hypotheses under natural conditions at the field scale. These sites also provide access to DOE site locations exhibiting complex geology and contaminated/uncontaminated areas where scientists can conduct short-term, field-scale research and obtain DOE relevant samples of soils, sediments, and groundwater for laboratory research. Information about these three projects can found in the links below.

Oak Ridge - http://www.esd.ornl.gov/orifrc/index.html

Old Rifle - http://ifcrifle.pnl.gov/

Hanford 300 Area - http://ifchanford.pnl.gov/

Other DOE facilities/resources that are integral to ERSD research include:

- **DOE Synchrotron Light Sources.** ERSD provides user support for experiments that require structural and chemical information often unavailable with conventional sources of x-rays.
- **Environmental Molecular Science Institutes (EMSIs).** ERSD and the Chemical Sciences, Geosciences, and Biosciences Division of the DOE Office of Basic Energy Sciences have teamed with the National Science Foundation to support the EMSI program, which is aimed at increasing the fundamental understanding of molecular-level process in natural environments, including those impacted by human activities. ERSD currently supports National Laboratory participation in three EMSIs, based at Stony Brook University, Pennsylvania State University, and Stanford University.
- **DOE High-Performance Computing Centers**, including the National Energy Research Supercomputing Center (NERSC) at Lawrence Berkeley National Laboratory and the Center for Computational Science (CCS) at ORNL.

The DOE sites across the U.S. also may serve as unique resources for obtaining relevant environmental samples, field experimentation, and concept validation. These sites contain more than a 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 NAPLs and their mixtures. ERSD research programs typically focus on representative contaminants and mixtures most critical to environmental remediation and site stewardship, including

- Radionuclides: plutonium, strontium-90, cesium-137, technetium-99, iodine-129, neptunium-237, and uranium
- Non-radioactive metals: chromium and mercury
- 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/)
- Savannah River Site (http://www.srs.gov/general/srs-home.html, http://www.srs.gov/general/enviro/erd/extpage.html).

In addition, ERSD supports research coordinators at several DOE sites to help investigators network with the user community and ensure that that ERSD research is relevant to DOE's cleanup problems. A list of site representatives is available from ERSD (http://www.sc.doe.gov/ober/ERSD_top.html).

6.0 ERSD Linkages

Complementing available resources and other specialized resources above, the ERSD maintains strong liaisons within DOE and with other federal agencies and non-governmental organizations. Some examples of ERSD coordination with these organizations are given below.

6.1 Coordination Within DOE

Office of Biological and Environmental Research (BER) residing within BER and DOE-SC, ERSD is closely aligned with strong fundamental science programs at the interface of the biological, physical, and computational sciences. The multidisciplinary nature and goals of ERSD reflect this strong BER tradition. Among the other BER divisions and programs are several opportunities to strengthen and extend ERSD programs.

The **Genomics: GTL program** within the **Life Sciences Division** initially is focusing on microbial genomics, an increasingly important area of research in environmental remediation. Bacteria and microbes impact most geochemical process, including rock weathering, contaminant fate, and mineral synthesis and dissolution. Likewise, the study of microbial genomics will be most meaningful when understood in the context of the natural environment where physical and geochemical properties and processes can exert marked influences on microbial communities and their activity and metabolism. It is therefore expected that ties between ERSD and Genomics: GTL will grow stronger as both programs develop.

The Joint Genome Institute (JGI) has been responsible for sequencing genomes of a number of microorganisms important to understanding contaminant fate and transport in the environment and to developing new concepts for *in situ* remediation of contaminated subsurface systems. The continued development of high-throughput functional genomics at JGI and the construction of the Genomics: GTL user facilities will result in incredible new tools for interrogating microbial environmental diversity and system level responses and function at the molecular, cellular and community levels.

Research in **Low Dose Radiation** provides a new scientific basis for determining the health risks from low doses of ionizing radiation that will be important to ERSD as risk-based approaches are increasingly used to direct, focus, and assess the efficacy of environmental remediation at DOE sites.

The Climate Change Research Division shares with ERSD an interest in multimedia transport issues. Investigations directed toward simulation of air-land-ocean interactions face problems similar to those faced in modeling reactive transport of chemical species in subsurface media. Moreover, regional changes in precipitation patterns that result from global climate change have the potential to affect both the transport of contaminants by surface and near-surface hydrologic systems, as well as the availability of potable water, both of which are issues of interest to ERSD programs.

ERSD and the **Medical Sciences Program** share a strong interest in research into new imaging modalities.

Office of Basic Energy Sciences (BES) research programs in **geosciences, heavy element chemistry and separations, materials science, and energy biosciences** complement ERSD research in understanding critical environmental processes. BES is responsible for the construction and operation of many of the large-scale experimental user facilities that have become essential tools for ERSD researchers. In particular, the availability of the BES-operated **synchrotron X-ray light sources** has greatly enhanced the ability to probe the chemical speciation of contaminants in the environment. Environmental science is now the fastest growing area of application for the light sources. ERSD will continue to work closely with existing BES programs and to seek opportunities for new linkages with emerging BES initiatives, such as the **Nanoscale Science Research Centers** and the **Spallation Neutron Source**, which currently are under construction.

ERSD is working closely with the **Office of Advanced Scientific Computing Research (ASCR)** to help ensure that the best available computational capabilities are directed toward reliable prediction of field scale subsurface contaminant behavior and the response of these systems to remediation. Fully competent predictions will form the basis for decisions on environmental stewardship and the protection of human health with long-term implications for U.S. environmental and energy policy. In addition, the two offices closely coordinate high-end computational resources to limit duplication of efforts in EMSL and ASCR computational facilities. Subsurface modeling has been identified by ASCR as a critical area for advanced computing research.

6.1.1 DOE Mission Offices

ERSD interfaces with the DOE field offices and contractors, the **DOE Office of Environmental Management** (EM), and other DOE mission offices concerned with preventing, treating, or controlling environmental contamination. ERSD will build on and expand the relationships that EMSP, NABIR, and SREL have established with the cleanup sites. Joint ERSD/EM review of new ERSD notices helps ensure that ERSD solicits and supports fundamental science most relevant to DOE site problems. In addition, close liaisons are developing between ERSD and the **DOE Office of Legacy Management** (LM). ERSD field research at UMTRA sites to assess potential biological solutions to uranium mobility has involved close coordination and review by LM.

Research on waste processing and waste form performance are highly relevant to the **DOE Office of Nuclear Energy, Science, and Technology's** Advanced Fuel Cycle Initiative, which seeks to develop reprocessing and fuel treatment technologies that are cleaner, more efficient, less waste-intensive, and more resistant to proliferation.

6.2 Coordination with Other Federal Agencies and Non-Government Organizations

6.2.1 Federal Agencies

ERSD objectives for interacting with other federal agencies and the larger environmental remediation communities generally are twofold. First, through these interactions, ERSD can leverage limited resources by collaborating on common or complementary interests. Second, these interactions allow ERSD to help coordinate and strengthen federal programs applicable to environmental remediation at DOE sites. ERSD's principal interactions are with the **National Science Foundation** (NSF), **U.S. Environmental Protection Agency** (EPA), and the Strategic Environmental Research & Development Program (SERDP).

Coordination with other agencies also is facilitated through the National Science and Technology Council's (NSTC) Committee on Environment and Natural Resources (e.g., the Toxics and Risks and the Water Quality and Availability Subcommittees), the Committee on Science (e.g., Interagency Working Group on Environmental Biotechnology), and the **Interagency Working Group on Multimedia Environmental Models** that has provided technical insights critical to the design and implementation of ERSD research to improve the development of conceptual models for subsurface contaminant transport and remediation.

6.2.2 Non-Government Organizations

A key ERSD connection with the National Academies is through study projects performed by **National Research Council** (NRC) committees overseen by the Board on Radioactive Waste Management. This body has played a major and longstanding role in critical review of scientific issues associated with the remediation and stewardship of DOE sites. Other NRC bodies of interest to ERSD program areas include the Board on Chemical Sciences and Technology, Board on Earth Sciences and Resources, Water Science and Technology Board, and the newly formed Western Water Resources Coordinating Council.

Scientific professional societies represent an important nongovernmental source of information, resource networking, and advisory talent for ERSD programs. Societies with which DOE-SC has longstanding ties include the American Association for the Advancement of Science (AAAS), American Chemical Society (ACS), American Society for Microbiology (ASM), American Physical Society (APS), American Geophysical Union (AGU), Soil Science Society of America, and the Materials Research Society.

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ERSD home page: http://www.sc.doe.gov/ober/ERSD_top.html

8.0 References and Related Websites

Allen, R.W., G.B. Johnson, J.H. Westsik, and C.L. Nickola. 2001. *Tanks Focus Area Site Needs Assessment*. PNNL-13518, Pacific Northwest National Laboratory, Richland, WA. (http://www.tanks.org/DocumentSearchResultsSingle.asp?DocumentID=4419)

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, and A.E. White. 2004. "Proposed Initiative Would Study Earth's Weathering Engine." *EOS* 85, 265-269.

Crowley, K.D and J. F. Aherne. 2002. "Managing the Environmental Legacy of U.S. Nuclear Weapons Production." *Amer. Scientist*. (Online) 90: 514-526.

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

DOE. 1997. *Linking Legacies: Connecting the Cold War Nuclear Weapons Production Processes to Their Environmental Consequences*. Office of Environmental Management (DOE/EM-0319) U.S. Department of Energy, Washington, DC. (http://legacystory.apps.em.doe.gov/index.asp)

DOE. 1999. *From Cleanup to Stewardship*. Office of Environmental Management (DOE/EM 0466), U.S. Department of Energy, Washington, DC. (http://lts.apps.em.doe.gov/center/companion.asp)

DOE. 2001. *Long-term Stewardship Study*. Office of Long Term Stewardship, U.S. Department of Energy. Washington, DC. (http://lts.apps.em.doe.gov/center/stewstudycontent.html)

DOE. 2004a. *Office of Biological and Environmental Research Environmental Remediation Division Draft Strategic Plan* (Available by request from the Environmental Remediation Science Division SC-23.4/Germantown Building, U.S. Department of Energy, 1000 Independence Ave., SW, Washington, DC 20585-1290).

DOE. 2004b. *A Science-Based Case for Large Scale Simulation. Vol. II.* Office of Science, U.S. Department of Energy. Washington, DC.

DOE. 2006. *Bioremediation of Metals and Radionuclides: What It is and How It Works – 2nd Edition.* Office of Science, U.S. Department of Energy, Washington, DC.

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://darwin.nap.edu/books/0309066468/html/R1.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://darwin.nap.edu/books/0309075602/html/24.html).

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

National Research Council. 2003, *Long-Term Stewardship of DOE Legacy Waste Sites: A Status Report.* Washington DC, National Academy Press. (Available at http://www.nap.edu/catalog/10703.html)