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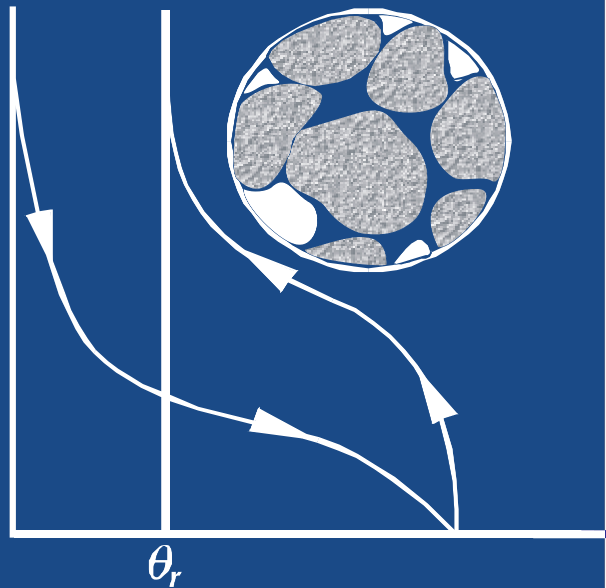


A National Roadmap for Vadose Zone Science & Technology

Understanding, Monitoring, and Predicting Contaminant Fate and Transport in the Unsaturated Zone

Revision 0.0

August 2001

PREFACE

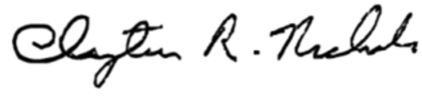
The project management and logistical aspects of initiating a first national roadmap for vadose zone science and technology are daunting. The initial challenge was to select and assemble a team of experts who could identify the research and development needed over the next quarter century to adequately assess and predict the fate and transport of contaminants in the vadose zone. The second challenge was to ensure that the group was well-versed in U.S. Department of Energy (DOE) needs, the vadose zone cleanup efforts of other federal agencies, and the research underway in universities, the private sector, and government facilities (including the DOE national laboratories). Third, the interests and requirements of federal, state and local governments had to be considered.

After a lengthy search, 10 internationally recognized individuals were selected and accepted positions on the Vadose Zone Roadmap Executive Committee. Four of these individuals also accepted the challenge to serve as workgroup chairs and to assemble the remainder of the participants for the workgroups. The full team consisted of 62 individuals, many of whom are internationally recognized vadose zone experts. These individuals (a complete list is provided in Appendix A) also provided representation from across DOE, other federal agencies, industry, academia, and the international community.

In March 2000, the Executive Committee met to begin its task. Over the next year, this committee and four (ultimately condensed to three) roadmap workgroups formed the multi-disciplinary team that has outlined in these pages a set of vadose zone research and infrastructure priorities for the next quarter-century.

As a starting point for this group, personnel from the DOE national laboratories who are familiar with end user needs and vadose zone issues (including several key collaborators developing the compendium *Vadose Zone Science and Technology Solutions*) prepared a summary of current deficiencies and capability gaps, within the DOE complex, in vadose zone characterization, monitoring and modeling. The results of this effort were provided to the roadmap team. During the second half of the year, the scope of the roadmap was broadened from a focus on DOE problems and needs to a national perspective on vadose zone contamination as a threat to our invaluable groundwater resources.

This roadmap is drawn in broad strokes. It no doubt leaves important research needs and opportunities uncharted. Nevertheless, it provides the first attempt at a national level to forge a path through what had been unmapped territory. If successful, the research described in this document will dramatically improve characterization, monitoring and modeling capabilities. These capabilities will provide a firmer scientific foundation upon which regulators and site managers can make confident decisions and predictions when dealing with contamination in the vadose zone. Additional work to refine, extend, and update this roadmap will require continued dialogue within the vadose zone research community, with other U.S. government and state and local agencies, and with affected stakeholders.



– Clayton R. Nichols, Assistant Manager, Research and Development;
U.S. Department of Energy, Idaho Operations Office

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FOREWORD

This roadmap is a means of achieving, to the best of our current knowledge, a reasonable scientific understanding of how contaminants of all forms move in the vadose zone, in the principal geological environments. This understanding is needed to reduce the present uncertainties in predicting contaminant movement, which in turn will reduce the uncertainties in remediation decisions.

The roadmap does not assign a value to the information needed, nor does it express in quantitative terms how much would be saved, were the information in hand. It does not discuss tradeoffs in remediation techniques or the political and economic factors involved. Nor does it explore the use of decision analyses to determine the "best" means of remediating a site. Rather, the information obtained from the research proposed here will help determine the best course of action at the most recalcitrant sites of subsurface contamination in the United States and abroad. Achieving this ultimate objective will take some time, as fundamental knowledge is needed. However, there will also be significant value gained almost immediately from these undertakings.

For example, a number of the activities have, as their objective for the first four years, the transfer of our state-of-the-art knowledge of hydrogeologic processes and measurement technologies into the state of practice at priority sites of subsurface contamination. Accomplishing this transfer of knowledge into practice will improve decisions taken on remediation techniques almost immediately. In addition, encouraging bright young people entering the research community to take on the challenges presented here will permeate new ideas and approaches into the decision process on remediation techniques almost instantaneously.

For much of the twentieth century, subsurface hydrological scientists focused on groundwater to develop dependable water supplies. Except for some scientists in the agricultural sector, there was little interest in vadose zone hydrogeology until the past 20–30 years. Consequently, our understanding of contaminant migration processes in the vadose zone is often insufficient to make accurate predictions about the future. Past predictions of flow of contaminants through the vadose zone have been grossly in error, leading to lack of trust and excessive conservatism in design of remediation techniques (National Research Council, 2000). The purpose of a roadmap like this is to lead to better understanding quicker. Better understanding of vadose zone contaminant migration processes and improved tools for prediction will enable better (more effective and less costly) cleanups. With present knowledge and technology, satisfactory cleanup is not possible in all circumstances and confidence in future performance is often low. Even so, research is not a substitute for cleanup, and where effective solutions are currently possible, cleanup in progress must proceed.

At DOE and other federal facilities, remediation processes are already underway. However, there are still mysteries of how flow through the vadose zone occurs in some geological formations, such as karst and fractured rock, and difficulties remain in predicting, for instance, the transport of colloids and movement of non-aqueous phase liquids. Because of these and other limits on our understanding, unacceptable quantities of pollutants will remain at some sites, even after currently planned remediation. Therefore, while remediation should progress in accordance with agreements reached under the Federal Facilities Act, only incomplete remediation is possible with today's knowledge of subsurface conditions and flow. The research activities mapped out here are intended to reach a level of understanding that will enable satisfactory remediation at all sites of subsurface contamination.

Although this initial roadmap effort focuses on the problems of sites managed by DOE and other federal entities, these problems are a small subset of the water resource problems, both of quantity and quality, in the world today. There are increasing water demands and shortages. With just the present world population of 6 billion, the annual depletion rate of groundwater aquifers is 160 billion cubic meters (Brown, 2001). As a result of groundwater withdrawals for human uses, water tables in the High Plains Aquifer (e.g. Ogallala) have dropped by more than 150 feet, decreasing the saturated thicknesses more than 50 percent (Alley et al., 1999). This depletion of water resources can only increase with future population growth.

Water suitable for human and agricultural uses has been a crucial historical factor. Despite hurricanes and tornadoes, “more than any other weather or climate event, the 1930s drought shaped American society. …. At its height in July 1934, nearly two-thirds of the nation was considered to be in severe to extreme drought” (Henson et al., 1999). The National Drought Policy Commission (2000) reported that “drought occurs some-where every year in the United States. It can and does extend over long periods and large areas, and it brings hardship.” For instance, the 1998 drought in Texas cost $11 billion.

When water supplies were plentiful, water management in the United States was almost solely *supply* management. Now, water management is evolving to include optimal use, quality maintenance, and conservation. Protecting groundwater quality is particularly important because 40 percent of U.S. public water supplies, plus an additional 40 million people, derive their drinking water from groundwater (Solley et al., 1993). Thus, more than 50 percent of the U.S. population depends on groundwater for its drinking water. Monitoring the vadose zone to detect contaminant migration early is critical, as is preventing contaminated waters from passing through the vadose zone to groundwater aquifers.

In summary, the vadose zone is the key to the security of our groundwater resources. Through this permeable cover atop the groundwater table, rain and snow replenish our underlying aquifers. Contaminants migrating through the vadose zone threaten this resource. This roadmap for vadose zone science and technology is intended to give us the tools needed to describe and forecast accurately the processes controlling this natural recharge and the consequences of subsurface contaminants on our groundwater.

– Daniel B. Stephens, Chair Vadose Zone Executive Committee;
President, Daniel B. Stephens & Associates, Inc.

EXECUTIVE SUMMARY

The Context

The vadose zone comprises the region between the land surface and underlying groundwater aquifers. Until recently, disposing of waste solids and liquids in the vadose zone caused little concern because this seemed a safe way to contain the wastes and keep them relatively immobile. Discoveries of hazardous and radioactive chemicals migrating through the vadose zone and entering groundwater have changed many assumptions about the vadose zone and heightened the importance of understanding this complex region of the earth. We now know that the movement of water (or other fluids) through the vadose zone can transport many waste components to underlying aquifers. Once groundwater is contaminated, control of the contaminants becomes more difficult and costly. Impacts on human health and the environment can result, as the contaminated groundwater discharges into surface waters or is pumped to the surface for irrigation, drinking, or other uses.

The circumstances that the Department of Energy (DOE) faces in addressing uncertainties about contaminant movement in the vadose zone at its cleanup sites apply in varying degrees to other owners of vadose zone contamination problems and to environmental regulators. Our current ability to predict and optimally manage fluid flow and contaminant transport processes in the vadose zone is limited by inadequate understanding of processes that typically incorporate geological, hydrological, chemical, and biological processes and properties. There is a general lack of methodologies to adequately represent water flow and contaminant transport processes and properties in highly heterogeneous media across multiple spatial and temporal scales. These uncertainties and knowledge gaps are exacerbated by our general inability to simulate even known processes realistically, given limited data, or to simulate assumed processes with little data. The uncertainties in our understanding, our data, and our ability to monitor and model contaminant movement in the vadose zone have eroded public trust and greatly increased public expense.

In the late 1990's, DOE undertook a major review of the state of the art associated with the vadose zone. The result was *Vadose Zone Science and Technology Solutions*, a two-volume compendium of both the state of practice and the state of science in vadose zone characterization, monitoring, and modeling, as well as technologies for remediation and waste isolation. It also contains a series of recommendations on filling gaps in our knowledge of vadose zone properties and technologies. During this same period, science and technology (S&T) roadmaps for individual DOE sites were being prepared. These predecessor activities contributed substantially to developing this first national S&T roadmap for vadose zone characterization, monitoring, and modeling.

The Roadmap Activities

The technical content of the roadmap is captured in 61 activities, most of which have associated tasks and status points with either a near-term, mid-term, or long-term time frame for achievement. *Near-term* means roughly within 4 years of beginning roadmap implementation. *Mid-term* means the results can be expected within a decade. *Long-term* applies to results over two to three decades (roughly, a 25-year horizon). Each activity represents an area for which critical research objectives and application requirements can be clearly stated.

The narrative to describe and support the 61 activities is divided into five major sections:

- Section 1 introduces the rationale for undertaking this effort, including the scope of the problem at DOE sites and elsewhere, the background of previous work on which this roadmap builds, and the Executive Committee's vision of what could be achieved, if the roadmap activities are implemented.
- Section 2 describes research and application activities to improve the understanding of basic physical, chemical and biological processes and properties, as well as improving the modeling, measuring, and monitoring of flow and transport.
- Section 3 identifies and discusses activities for cross-cutting issues, such as coupled processes, scaling, measuring and reducing uncertainty, advances in site monitoring systems, and the integration and validation of characterization, monitoring, and assessment tools at the system (field scale) level.
- Section 4 focuses on the infrastructure and capabilities required to accelerate progress along the activity pathways identified in Sections 2 and 3.
- Section 5 presents general conclusions and recommendations from the Executive Committee, including a summary review of major near-term, mid-term, and long-term results that it anticipates will follow from pursuing the roadmap, key linkages among the activities, and the importance of broad cooperation and coordination if the goals of the roadmap are to be achieved.

In many instances, early results from the research activities described in the roadmap, particularly application status points, are prerequisites for a supporting capability or infrastructure element. These capabilities and supporting elements, in turn, enable and accelerate the more advanced work along the research activities. Key elements of infrastructure and supporting capability include:

- A national virtual library of geological, hydrologic, chemical, and biological data from major sites of vadose zone contamination, together with prototype numerical models designed to work with these multidisciplinary datasets.
- Advances in sensor instrumentation, particularly in miniaturization (packaging) and emplacement technology.

- Advances in design and optimization of sensor networks for monitoring and characterization.
- Facilities to support integrated testing and validation of vadose zone research.
- A problem-solving software environment developed specifically for vadose zone modeling and analysis tasks.
- Advances in numerical algorithms directed at difficult vadose zone computational problems.
- A high-power computing capability dedicated to vadose zone applications and related environmental S&T issues.

Anticipated Results

Many of the near-term results expected for both the research and infrastructure activities share a common theme: *moving the state of the art to the state of practice*. This means getting the current knowledge and capabilities already existing in the research communities into operational use at the nation's priority sites of vadose zone contamination. One benefit is that these tasks "pick the low-hanging fruit," providing quick returns because much of the research investment has already been made. A less obvious benefit is that concerted effort to get new knowledge and technical capability into practice will bring researchers and solution-oriented problem owners into continuing and close interaction.

For the mid-term, the roadmap outcomes of greatest significance are likely to be the cumulative *advances in monitoring systems* for vadose zone sites. A sound and efficient monitoring program is critical at major sites during environmental cleanup and afterward, throughout any period of stewardship required by residual contamination on site. The state of practice has been to monitor the groundwater at and around the site, rather than monitoring the vadose zone. However, for many sites where contaminants are at some distance from the water table, waiting until contaminants appear in the groundwater is less desirable than monitoring the vadose zone. If remediation can remove or isolate source terms and halt plumes while they are still in the vadose zone, groundwater contamination can be prevented. In addition, the effectiveness of the remediation is often greatly enhanced, and the cost significantly reduced, compared with groundwater remediation alternatives.

Many of the long-term results anticipated from the roadmap activities will provide *better tools for supporting site-wide assessments and decisions* on environmental cleanup and stewardship. Models and data gathering will undoubtedly improve incrementally in the near and mid-term. However, after a decade or so of pursuing the roadmap's activities, a qualitative leap forward is expected in the ability to visualize, quickly and accurately, the current and projected future states of site-wide vadose zone systems. These projections, which will carry levels of certainty and sensitivity unattainable at present, should suffice to win the confidence of regulators and the public.

How the Roadmap Links to Environmental Cleanup and Stewardship

This roadmap covers only a part of the effort needed for environmental cleanup and stewardship of the nation's vadose zone contamination problems. It does not cover the S&T for remediation and isolation techniques or other modes of action for exercising stewardship in the broadest sense. Nor does it include the S&T to support assessment of impacts on human health, the environment, and the local, regional, or national economy. Nevertheless, results of activities in this roadmap will affect S&T activities for contaminant removal, immobilization, or other cleanup operations, as well as choices among cleanup and attenuation options. Progress in the S&T for remediation activities will in turn influence the work needed in site visualization and monitoring systems, sensor and measurement techniques, and even the amount of understanding needed about various vadose zone processes. More broadly, achieving near-term results will influence the support from stakeholders and government budgeting authorities for further efforts to understand, monitor, and control contaminants in the vadose zone. In this light, it is important that this roadmap be integrated with the larger context of S&T planning for cleanup and stewardship.

Given the broad potential applicability of the S&T work identified here—and the sheer scale of the effort that implementation will require—a coordinated approach involving many federal agencies is essential. From this perspective, the current version of the roadmap is unquestionably a first step for consideration and revision in a context where the other agencies are more fully involved as partners with the DOE.[1] There should also be some mechanism to represent State and local entities in the process because of their growing importance in oversight of and decisions about environmental cleanup and stewardship.

Whenever the resources needed for a range of potential activities are limited, there is potential for competition among those activities. However, focusing on just the potential for resource competition between vadose zone research and ongoing cleanup operations ignores the considerable potential for constructive influences and synergies, which a systematic approach to resource allocation can tap. *A well-planned program for research and development to improve cleanup and stewardship options can, and should, be a profitable return on investment for the nation.* The ultimate driver for significant investment in the research and infrastructure activities contained in this roadmap is to protect an even more valuable national treasure, our groundwater resource.

[1] However, this report was developed by a broadly representative group of researchers. The Executive Committee included representatives of the agencies most likely to be involved in a coordinated national effort.

1.0 INTRODUCTION

1.1 The Need for a Better Understanding of the Vadose Zone

The vadose zone comprises the region between the land surface and underlying groundwater aquifers. Although technically water in the vadose zone is water in the ground, we shall adhere to the classical definition of groundwater as "subsurface water that occurs beneath the water table in soils and geological formations that are fully saturated" (Freeze and Cherry, 1979). Across the United States, activities by individuals, companies, and state and local governments, as well as by federal government agencies, have resulted in the release of contaminants at or near the land surface. Underground waste burial, landfill dumping, and direct discharge of liquids to the soil surface were generally accepted practice for disposal of a wide range of wastes. These wastes were, until recently, believed to be relatively immobile and thus were viewed as not being a potential source of aquifer contamination. The prevailing wisdom held that retention in the vadose zone, decomposition (of chemical and organic wastes), or dilution to a vanishingly low concentration would keep us safe. As a result, little attention was given to understanding the nature of the vadose zone, the potential pathways for fluids or contaminants to disperse throughout the zone, or the myriad possible interactions among fluids; contaminants; and the chemical, biological, and physical components of the vadose zone.

We now know that the movement of water (or other fluids) through the vadose zone can transport many waste components to underlying aquifers. From there, groundwater movement can carry them to springs, streams, lakes, rivers, and coastal waters. Wells can pump wastes in the aquifer back to the surface, where environmental and human exposures can occur. Discoveries of hazardous and radioactive chemicals migrating through the vadose zone and entering groundwater have changed many assumptions about the vadose zone and heightened the importance of understanding this complex region of the earth.

In the absence of adequate predictive capabilities, the ability to detect contaminant migration and fate early is all the more critical. Extensive field experience and theoretical considerations have demonstrated that remediation costs and risks increase exponentially as contaminated volumes increase and concentrations decrease. From a containment/remediation standpoint, detecting contaminant migration when it is still in the vadose zone—before it reaches underlying and downgradient groundwater—provides the best opportunity (short of preventing releases in the first place) for less-difficult actions at lower cost and risk. Recent reports by the National Research Council address this point. The authors of one study concluded that pump and treat technologies are inefficient for remediating contamination in groundwater. This conclusion supports the argument that intervention while contaminants are still in the shallow vadose zone is preferable to waiting until they have migrated into aquifers or to greater depths.[2,3]

Before intervention can be undertaken, even before one can decide which intervention approach is best, subsurface contaminants must be identified. Their nature and extent must be determined. The physical, chemical, and biological properties of that specific vadose zone environment must be ***characterized*** well enough to know whether, how, and how fast the specific contaminants will be transported by fluid movement through the vadose zone. While remediation activities are being planned and implemented, the vadose zone within and around the contaminated volume must be ***monitored*** to determine whether and where contaminants are moving. If the chosen remediation approach leaves contamination in the vadose zone (which will be inevitable in many instances), continued monitoring of the site is often essential. Given the complexity of the vadose zone environment and of the interactions between this environment and contaminants, computer-based ***modeling and simulation*** are essential aids in understanding vadose zone processes and contaminant transport, including visualizing existing and potential conditions at a contaminated site.

1.2 A Broad National Issue; a Department of Energy Mission

Threats to valuable, often irreplaceable, groundwater resources from contaminants in the vadose zone occur nationwide. They arise from a remarkably diverse range of human activities. Leachate from municipal or commercial landfills and leaks from abandoned or aging underground fuel tanks and piping pose problems in every region, as do industrial dump sites and process waste burial grounds. In agricultural areas, pesticides, fertilizers, pathogenic organisms, and spilled or dumped fuels can be transported to groundwater, sometimes threatening the principal source of water for irrigation and other commercial uses, as well as the drinking water for humans and livestock (see accompanying textbox on agricultural herbicides). In some suburban areas, increasing household density and water consumption, particularly where homes use septic tanks with leach fields, are straining the biodegradation capacity of subsurface microbial and geochemical systems. The same is true for pathogenic microorganisms and pharmaceuticals being released from animal wastes.

On military bases around the country, landfills, burial sites, and waste handling or storage areas on the surface often contain hazardous materials in larger quantities and of different types than those in a municipal landfill or typical industrial waste site. Firing ranges and old ammunition dumps may contain ordnance and related materials whose chemical components pose a vadose zone contamination hazard, as well as a safety hazard for cleanup crews.

[2] "Alternatives for Ground Water Cleanup" in *Technologies for Environmental Management: Summary of a Workshop*, National Research Council, 1997, p. D-111

[3] *Groundwater and Soil Cleanup: Improving Management of Persistent Contaminants*, National Research Council, 1999, p. 3

Another major consequence of preparations for national defense during the past half-century are sites around the nation where large-scale production or processing of nuclear materials were accompanied by planned and unplanned releases of process wastes to the subsurface. The Department of Energy (DOE) and its predecessor agencies have conducted energy research and weapons development and production at facilities in 31 states and Puerto Rico. Toxic chemicals generated at these sites have been introduced into the underlying soils and aquifers as a result of a number of historical and current practices. At present, more than six billion cubic meters of subsurface media at 134 sites are contaminated.[4] Of this, approximately 700 million cubic meters is groundwater contaminated with organic wastes (e.g., solvents, fuels, polychlorinated biphenyls),

Herbicides Detected in the Nation's Groundwater

The U.S. Geological Survey is conducting the National Water-Quality Assessment (NAWQA) program to measure the concentrations of a large number of pesticides, pesticide transformation products, and other chemicals in groundwater, surface water, stream sediments, and aquatic plants and animals (biota). Eventually the NAWQA program will cover 59 major hydrologic basins across the United States, representing 60 to 70 percent of the nation's water use. Results from the first three years (1993-1995) of intensive sampling in 20 of the basins were summarized in the May-June issue of the *Journal of Environmental Quality* (Barbash et al., 2001). This summary report focuses on the frequency of detection of seven herbicides. Six of the herbicides (atrazine, cyanizine, simazine, alachlor, acetochlor, and metolachlor) are high-use agricultural herbicides; the seventh, prometon, is a nonagricultural herbicide.

The samples, taken from both shallow and deep wells, rarely exceeded the quality criteria for drinking water set by the EPA. In only two samples, both from shallow groundwater, did any of these seven pesticides exceed the maximum concentration limit (MCL). In both instances, the herbicide was atrazine, the herbicide most frequently applied in the United States prior to the sampling period. Atrazine was also the herbicide most frequently detected[a] in shallow groundwater in agricultural areas (detected in more than 30 percent of the samples) and in deep ground water (detected in about 7 percent of samples). Prometon was the herbicide detected most frequently in shallow groundwater in urban areas (24 percent), with atrazine second (14 percent). The authors concluded that the frequency of use of an herbicide correlates with its frequency of detection in shallow groundwater. Statistical analyses of the data (by multiple regression) found that frequency of use of the pesticide and its half-life in the soil under aerobic conditions were significantly correlated with frequency of detection. However, these two variables together accounted for less than 40 percent of the variability in detection, which the authors interpreted to mean that additional factors are involved.

The above data show that once pesticides are applied to the soil surface, or incorporated into the upper soil horizons, they may not remain there but can travel through the vadose zone to underlying groundwater resources. Their fate and transport in the vadose zone is determined by a plethora of physical, chemical and biological processes such as those discussed in this roadmap. Downward transport actually can be very rapid. For example, the U.S. Geological Survey also detected the pesticide acetochlor in several samples. Acetochlor was first licensed for use in the United States in 1994 and first applied in agricultural areas in June of that year. By the following year, the NAWQA program detected this pesticide at two of its 991 shallow groundwater sampling sites. The timing of these observations supports earlier field-scale studies suggesting that pesticides can move rapidly through the vadose zone and appear in shallow groundwater within a year following first application.

[a] All frequencies of detection cited here are for a detection limit of 0.01 microgram per liter.

[4] *Research Needs in Subsurface Science*, National Research Council, 2000, pp. 15 & 21

radioactive waste, or mixed (chemical and radioactive) waste. Today, some 60 million cubic meters of soil and rock within the vadose zone are contaminated, mostly with radioactive waste or mixed low-level radioactive waste.[5] Cleaning up these sites is a DOE responsibility. Where the current plans for cleanup will leave subsurface contaminants in place, long-term stewardship of the site will be needed.

There is substantial commonality among the basic processes at work across all these diverse circumstances of vadose zone contamination. Understanding vadose zone processes and being able to measure, monitor, and predict the subsurface movement of contaminants at one site, for example a DOE site, can aid in addressing problems where contaminants from other human activities have entered similar subsurface environments. This commonality in vadose zone environments, coupled with the national interests at stake in protecting our groundwater resources, calls for a cooperative, coordinated effort among the various federal and other entities engaged in vadose zone research.

While DOE is far from being alone in "owning problems" of vadose zone contamination, it certainly has the responsibility for some of the nation's most contaminated sites. The radiological hazards present at many of the contaminated DOE sites, as well as the sheer volume of wastes still in storage or in the subsurface, create special, and sometimes unique, requirements for characterization, monitoring, and modeling. The central importance of environmental cleanup and stewardship to DOE's mission, the scale of the effort required at some sites, and the commitment to solve the problems place it in a leadership role among problem owners.

1.3 The Need for a Vadose Zone Science and Technology Roadmap

1.3.1 Science and Technology Roadmapping

Science and technology roadmapping is a form of strategic technology planning used by an increasing number of companies, industries, and U.S. government agencies. The purpose of a science and technology roadmap is to develop a common perspective on possible future science and technology needs, in an effort to help make better research and development (R&D) investment decisions. Science and technology roadmaps are intended to serve as pathways to the future. They call attention to the underlying science and applied technology needed to solve currently intractable problems, provide a structure for organizing technology forecasts and programs, and communicate scientific and technological needs and expectations among end-users and the R&D community.

This *National Roadmap for Vadose Zone Science and Technology* focuses on research that will improve predictions of fate and transport of contaminants in the vadose zone, and thus reduce uncertainty in decisions made by both problem owners and regulators. In addition to the DOE, problem owners that could benefit include the Department of Defense (DOD), other federal agencies, state and local entities with responsibility for cleanup of contaminated sites, and perhaps even corporate and

[5] *Vadose Zone Science Integration and Technical Basis (DRAFT),* INEEL, 2000, p. 4

individual owners of serious subsurface contamination problems. The regulators include the U.S. Environmental Protection Agency (EPA) and the various state regulatory agencies responsible for human health and the environment. Another major focus of this research is to provide better tools for communicating the scientific basis of cleanup or stewardship decisions to stakeholders, those who are or could be affected by the consequences of vadose zone contamination and by the decisions made by problem owners or regulators.

1.3.2 Why the DOE Needs a Roadmap for Vadose Zone Science and Technology

Contaminants have been detected underground at unanticipated levels far from the point of release. The principal driver for the DOE in initiating a roadmapping process for vadose zone science and technology was the detection of contaminants that had been transported through the vadose zone much more quickly than the DOE had anticipated. Clearly, the assumption of vadose zone immobilization of contaminants was wrong. A better basis is needed for DOE's cleanup and stewardship programs.

Recent evidence indicates that hazardous and radioactive chemicals have migrated unexpectedly through the deep vadose zone at multiple DOE facilities. For example, at the Hanford 200 West Area Tank Farm, cesium-137 appears to have migrated roughly 80 feet vertically below the tank through highly sorptive material which should have prevented such migration. At Los Alamos National Laboratory, plutonium and americium were discovered 100 feet beneath a liquid waste impoundment where nuclide transport was believed to be dominated by sorption and thus where radionuclide migration should have been very limited. At Sandia National Laboratories, trichloroethane from a landfill was discovered at depths of 500 feet in an area of very dry soil and low recharge. Near the prospective site for a high-level radioactive waste disposal repository, in the dry desert climate of Yucca Mountain, tracer substances such as bomb pulse chlorine-36 and tritium, were found in fractured tuff at depths of as much as 1200 feet. These data imply unexpectedly rapid recharge along preferential pathways.

Information of this type led the authors of a National Research Council review of DOE's long-term stewardship program to conclude that there are "…deficiencies in our ability to make accurate estimates of subsurface contaminant behavior, especially in the conceptual understanding of this behavior to enable accurate and robust modeling."[6] This conclusion echoes a report by the Government Accounting Office (GAO) on contamination at the Hanford site. The GAO report concluded that DOE could not predict contaminant fate and transport in the subsurface with the certainty required to make key environmental decisions.[7]

DOE's Cleanup Timetable Is Driving the Need for Long-Term Stewardship Capabilities. Over the next 50 years DOE expects to complete cleanup activities at all of

[6] *Research Needs in Subsurface Science*, National Research Council, 2000, p. 53

[7] *Nuclear Waste: Understanding of Waste Migration at Hanford is Inadequate for Key Decisions*, Government Accounting Office, 1998

its sites and move from active remediation to ensuring long-term stewardship of these sites. Recent DOE documents define long-term stewardship as "…all activities required to protect human health and the environment from hazards remaining after cleanup is complete."[8]

Figure 1 illustrates the timeline by which DOE anticipates completing cleanup, and commencing long-term stewardship across 144 sites.[9] While DOE estimates that only about 123 sites will have been cleaned up and put in active or passive stewardship by the year 2006, all 144 sites will be so by 2050. Most of these sites, including the most complex ones, are located in semi-arid western states with thick vadose zones. The timeline driving DOE's cleanup mission, coupled with the prevalence of thick vadose zones at important sites, further dictates the need for an aggressive, accelerated program to understand vadose zone processes and properties, develop better tools and techniques to characterize and monitor contaminant migration and fate, and develop predictive models to address and assess long-term stewardship needs.

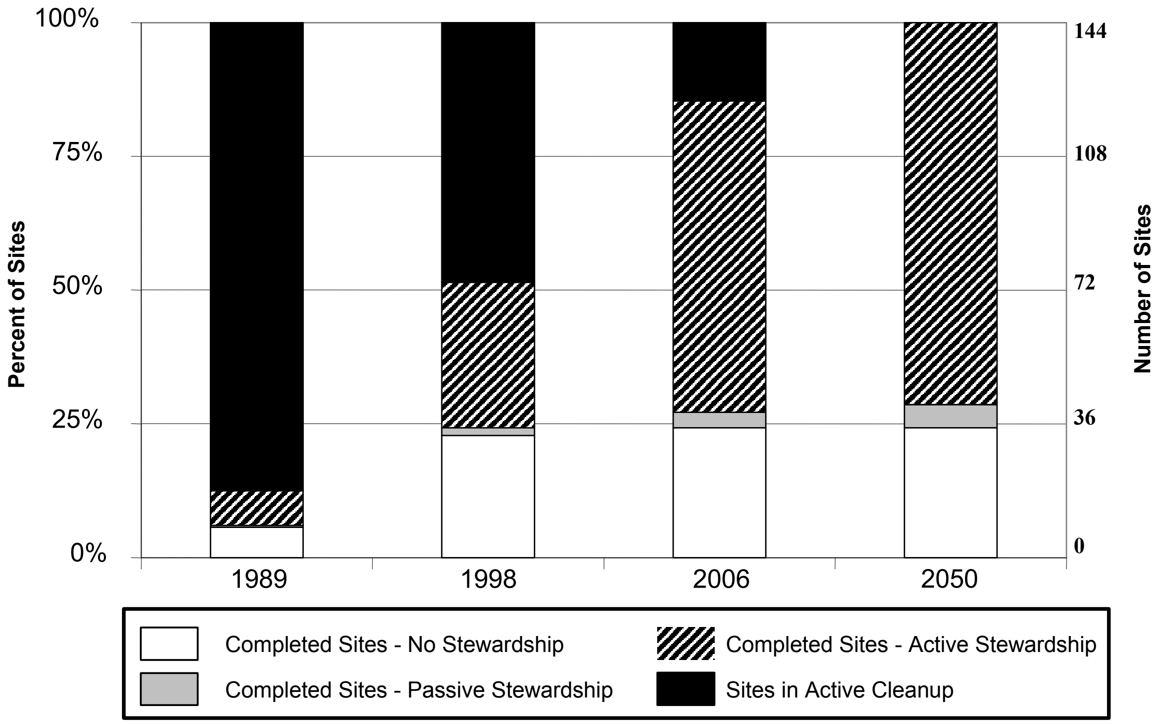

Figure 1 Stewardship Activities Increase as Cleanup is Completed

[8] *From Cleanup to Stewardship*, DOE, 1999b, p. 9.

[9] *Ibid.* p. 40. A cleanup site may be an entire facility, such as the Hanford Site, or a portion of a facility. The magnitude of contamination and extent of planned cleanup also varies greatly from site to site, as do the relative risks. For both reasons, Figure 1 should not be interpreted as indicating the magnitude of cleanup accomplished or remaining to be done at a given time, nor the decrease in risk over time.

1.3.3 The Need for a National Roadmap

Predictive models for fate and transport of contaminants in the vadose zone leave large uncertainties. The circumstances that the DOE faces in addressing uncertainties about contaminant movement in the vadose zone at its cleanup sites apply in varying degrees to other owners of vadose zone contamination problems and to environmental regulators. Our current ability to predict and optimally manage fluid flow and contaminant transport processes in the vadose zone is limited by inadequate understanding of processes that typically incorporate geological, hydrological, chemical, and biological processes and properties. There is a general lack of methodologies to adequately represent water flow and contaminant transport processes and properties in highly heterogeneous media across multiple spatial and temporal scales. For example, we are unable to measure state variables and parameters accurately, reliably, and in a timely fashion. We do not know how reliably the conceptual models for these processes, or the data used to define bounding conditions and parameters for a specific site, represent the actual processes and properties in the vadose zone.

These uncertainties and knowledge gaps are exacerbated by our general inability to simulate even known processes realistically, given limited data, or to simulate assumed processes with little data. In part, these simulation difficulties stem from the nonlinear parametric relationships that govern flow and transport through the vadose zone. In part, they are due to computational intractability posed by limitations in available hardware and software. Taken together, these various aspects compound the uncertainty within the models themselves. Simulation-induced uncertainties potentially amplify the gaps in our fundamental understanding of the processes being modeled and the uncertainties in our measurements of key properties. The development of the necessary process level understanding requires substantial advances in both instrumentation and in modeling capabilities.

No acceptable technical basis exists for regulatory oversight of the vadose zone. At many contaminated sites, contaminants have been released to the land surface, or have escaped gradually from buried containment systems, over a period of decades. Even at priority cleanup sites, leaking underground containers and long-buried wastes will continue releasing contaminants to the vadose zone for decades to come. For example, at the DOE sites with the largest quantities of waste, releases to the vadose zone will continue as a result of historical activities, planned containment, storage of new wastes in newly designed landfills, imperfect closure of contaminated buildings, abandoned contaminated subsurface piping, abandoned dirty facilities, and unexpected (as opposed to planned) future waste releases. This last category includes, for example, spills and leaks that will occur at facilities that will remain operational for the next several decades, prior to final closure. Not all of the contaminants can be removed from the surface or subsurface, and not only because the cost of removal is huge or because it is technically impractical to remove wastes hundreds of feet deep in highly heterogeneous media. In some circumstances, disposal of huge amounts of excavated materials containing low levels of contamination would simply shift the problem elsewhere.

The inability to explain basic subsurface processes fully and predict contaminant fate and transport in the vadose zone accurately has led some regulators to fall back on the most conservative expectations: all contaminants will move rapidly through the vadose zone to the groundwater. For example, in the late 1960s the time for carbon-14 to travel from the surface to groundwater at a site near the Idaho National Engineering and Environmental Laboratory (INEEL) was estimated at 80,000 years. Based on more recent measurements, the estimates are closer to 50 years.[10] Similar foreshortening of travel time predictions for other contaminants has also occurred. Despite these dramatic changes in expectations, many science and technology providers assert that the uncertainties in current predictions are just as great as the uncertainties in predictions made three decades ago.

To make regulatory and operational decisions regarding these long-term and continuing sources of contamination, the following questions must be addressed:

1. What quantity of existing contaminants must be removed?
2. How much residual waste can be placed in onsite landfills?
3. What kind of biogeochemical barriers can be used to enhance long-term entrainment (compared with hydraulic containment using a cover over the landfill)?
4. Will containment be necessary over the long-term, and if so, what kind?
5. What long-term geochemical transformations are expected in the containment facilities?

The research identified in this roadmap is necessary to provide the scientific foundation for answering those questions.

Uncertainties in predictions and in the basis for effective action create public distrust and misallocate limited resources. The uncertainties in our understanding, our data, and our ability to model contaminant movement in the vadose zone have two additional consequences: erosion of the public trust and greatly increased public expense. For example, at some DOE sites with thick vadose zones having low permeability, a waiver of groundwater monitoring in favor of vadose zone monitoring is an option under the Resource Conservation and Recovery Act (RCRA). However, regulators are reluctant to grant this variance because of uncertainties in the reliability with which vadose zone instrumentation can detect contaminants. Consequently, deep and often much more expensive groundwater monitoring is required.

Moreover, reliance on deep groundwater monitoring sidesteps the need to detect contaminants in the upper vadose zone, where their presence might trigger shallow soil remediation actions rather than expensive, difficult attempts to isolate and remediate

[10] For a further discussion of predicted contaminant travel times and how they have changed, see *Research Needs in Subsurface Science*, National Research Council, 2000, p. 30

contaminated groundwater at great depth. Finally, because of the large uncertainty in our ability to predict migration through the vadose zone and potential risks to groundwater users, engineered remedial measures are often designed with an excessive margin of safety applied to multiple design factors. These compounded safety margins in designs result in costly facilities—although the adequacy of the design may still be uncertain.

1.4 A Vision for 2025

Over the next few decades, dramatic and fundamental advances in computing, communication, electronics, and micro-engineered systems will transform many of the scientific and technical challenges we face today. For example, analytical systems that once would have required rooms of complex and fragile equipment are now located on a microchip. The computing power once reserved to put a man on the moon is now far surpassed by the power in a personal home computer. The technology trajectory expressed by Moore's Law, which predicts that microchip density doubles every 18 months, suggests that computing power may undergo more than a thousand-fold increase within the next 15 years.[11] Extended to the year 2025, this hypothesis implies that computing power may increase by more than a hundred-thousand-fold. With advances like these becoming commonplace, one can envision the following by the year 2025.

Our fundamental understanding of vadose zone properties and processes will be sufficiently developed, tested, and verified that issues of scientific uncertainty exert far less influence on public debates over interventions or on regulatory procedures to implement public policy.

In-situ and remote monitoring methods such as real-time detection and quantification of liquid and contaminant flow in fractures are widely used—and routinely accepted by problem owners, cleanup managers, regulators, and stakeholders—as an alternative to *in situ* sampling methods, such as groundwater monitoring. Using ultra-sensitive monitoring capabilities, investigators know whether liquid and contaminant migration is occurring within specific fractures or media.

A new generation of microscopic sensors, the size of grains of rice, can take simultaneous multichannel measurements (e.g., chemical species detection or pressure, temperature, pH and/or electromagnetic measurements) inexpensively and in real time. These sensors are small and inexpensive enough to inject into the material being investigated.

Vadose zone simulation and visualization capabilities compare in their complexity, speed, and accuracy to those used to model nuclear weapons systems and explosions, weather and climate, or molecular processes in biology. Access to these predictive and

[11] "Moore's Law" refers to the observation made in 1965 by Gordon Moore, co-founder of Intel, that the number of transistors per square inch on integrated circuits had doubled every year since the integrated circuit was invented. Moore predicted that this trend would continue for the foreseeable future. In the years since Moore made his prediction, this pace has slowed a bit, but component density has doubled approximately every 18 months.

interpretive tools revolutionize the way researchers, cleanup managers, and regulators think about the vadose zone and contaminant problems. These tools are routinely used to prepare site-wide assessments, with predictive scenarios for alternative courses of intervention, before major decisions on cleanup and stewardship.

1.5 The Context of Previous Vadose Zone Work

This roadmap represents the next phase in the historical evolution of technical and philosophical approaches to the vadose zone. The specific study of vadose zone hydrology is quite new, in fact the first graduate courses in this field were offered only in the early 1980s—just 20 years ago. When O. E. Meinzer wrote about the vadose zone in the first half of the twentieth century, he referred to it as “no man’s land” because of the lack of knowledge about its part in the hydrologic cycle (Looney and Falta, 2000, p. xix). Before 1980, most of those interested in studying the subsurface followed one of two paths, focusing either on groundwater hydrology or soil science. Groundwater hydrology has traditionally been a discipline of specialists trained in aquifer mechanics, well hydraulics, and groundwater basin management, mostly interested in groundwater supply issues. Soil physicists, whose academic discipline does include the study of water movement in the vadose zone, have focused on problems in irrigation and drainage of agricultural land. These fields of study evolved independently for the most part, although groundwater hydrologists often learned from the soil physicists and agricultural engineers to solve similar problems, recognizing for example, that the mathematical solution for flow to a drainage canal was similar to that for flow to a stream.

Today, however, driven in large part by the explosion in regulations to protect groundwater quality, hydrogeologists and soil scientists together are facing problems involving the flow of chemicals through the vadose zone to aquifers. The surge in environmental applications of soil science has led to interdisciplinary research sponsored by a wide range of state and federal agencies (Loaiciga et al., 1997; DOE, 1999a). Cross-training and cooperative research across multiple disciplines including hydrogeology, soil science, civil and environmental engineering, and petroleum engineering has been increasing dramatically, and a new field of vadose zone hydrology is now coming into its own. Major review articles and technical monographs on vadose zone hydrogeology and the flow and transport of contaminants in the vadose zone are proliferating.

In the late 1990's, DOE undertook a major review of the state of the art associated with the vadose zone hydrogeology. This activity resulted in the publication of *Vadose Zone, Science and Technology Solutions* (Looney and Falta, 2000). This two-volume compendium, which built upon four national meetings on various aspects of the vadose zone, was organized and led by DOE’s Savannah River Office. Within its 1600 pages, it identifies both the state of practice and the state of science in vadose zone characterization, monitoring, and modeling. Further, the national meetings and the collective efforts to assemble the compendium gave birth to a series of recommendations on filling gaps in our knowledge of vadose zone hydrology. As *Vadose Zone, Science and Technology Solutions* was being assembled and readied for publication in 1999–

2000, science and technology (S&T) roadmaps for individual DOE sites were also being prepared, for example at the Hanford Site and INEEL.

As a next step in DOE's effort to provide a better basis for its decisions on environmental cleanup and stewardship, DOE directed INEEL in 1999 to lead the development of an S&T roadmap identifying vadose zone research needed over the next 25 years. The scope of this roadmap was specifically restricted to understanding basic processes in the vadose zone and to techniques and technologies for characterizing, measuring, and modeling vadose zone processes and properties. Unlike the *Vadose Zone, Science and Technology Solutions* review or the site-specific S&T roadmaps, this roadmap effort would not address remediation approaches. In March 2000, an executive committee was formed to address the science and technology required for characterizing, monitoring, and modeling subsurface contaminant fate and transport. Over the next year, this committee and four roadmapping workgroups comprising sixty-two representatives from DOE, its national laboratories, other U.S. government agencies, universities, and industry discussed and agreed upon S&T capabilities that would transform the scientific basis for making decisions involving the vadose zone.[12] The resulting roadmap, presented in the following pages, delineates the critical research that must be conducted over the next 25 years to realize the vision of a sound scientific basis for making public policy and regulatory decisions. It also provides a structure for understanding the context of decisions being made on cleanup and long-term stewardship by DOE and the components that contribute to improved scientific input to these decisions with respect to the vadose zone.

If successful, the research described in this document will advance the state of the art in vadose zone characterization, monitoring, and modeling science and technology. To support the complex-wide needs of DOE, described above, as well as the needs of other owners of vadose zone contamination problems, and the regulators and stakeholders to whom they answer, these advances in the state of the art must make their way into advances in the state of practice. The work groups that developed this roadmap have emphasized pathways for this critical transformation of research results into practical results.

Creating a better scientific foundation for making both near-term remediation and waste handling decisions and long-term stewardship decisions regarding the management of contaminated vadose zone sites will require: 1) an enhanced understanding of basic subsurface processes; 2) adequate data on the properties of fluids and media that affect flow and transport in the vadose zone, the extent and character of existing contamination, and the ability to monitor it effectively; and 3) the ability to translate this understanding and data into new predictive models that can reduce the technical uncertainty in environmental management decisions. All three of these essential strands are woven through the fabric of the roadmap pathways and the supporting narrative.

[12] A complete list of participants is provided in Appendix A. The original sets of research goals formulated by the work groups are listed in Appendix C, which also indicates the roadmap activity, task, or status point corresponding to each research goal.

Activities, tasks, and status points are used to define roadmap paths. Section 2 describes the research and application activities to improve the understanding of basic physical, chemical, and biological processes and properties, as well as improving the modeling, measuring, and monitoring of fluid flow and contaminant transport. Section 3 identifies and discusses activities, tasks, and status points for cross-cutting issues, such as coupled processes, scaling, measuring and reducing uncertainty, and the integration and validation of characterization, monitoring, and assessment tools at the system (site-wide) level.

Each research activity outlined in Sections 2 and 3 represents an area for which critical research objectives and application needs can be clearly stated. For most activities, specific tasks and status points along the path of the activity are identified, and their relevance to achieving the activity's objectives is explained. A task represents work contributing to an ongoing activity but having a definite endpoint. The task endpoint can be considered the final status point for that task, indicating completion.

Supporting capabilities and infrastructure are needed to achieve research and application goals. Section 4 focuses on the infrastructure and capabilities required to accelerate progress along the activity pathways identified in Sections 2 and 3. In many instances, early results from these activities, particularly application status points, are prerequisites for phases in developing a supporting capability or infrastructure element. These capabilities and supporting elements, in turn, enable and accelerate the more advanced research activities. Thus, there is an iterative synergism between the activities in Sections 2 or 3 and those in Section 4. This synergism will be discussed further in Section 5.

The roadmap is structured into near-term, mid-term, and long-term time horizons. For this initial effort in defining roadmap paths, the work groups used three time horizons for tasks and status points. For the near-term horizon, the work groups aimed at efforts that could be completed in about 4 years (within a year or so of 2005). For a mid-term horizon of about a decade, the arbitrary time point was 2010. A long-term horizon of two to three decades was denoted by a time point of 2025. These arbitrary year dates should be understood as approximate markers for the three time horizons, near, mid, and long term, rather than as precisely scheduled milestones. As the roadmap evolves and the tasks and projects within an activity become better defined, more specific timing of results from the roadmap activities will become possible.

The activities and associated tasks and status points are listed in Sections 2 through 3 immediately following the narrative text that explains their value and the gaps they are meant to address. A complete table of all the recommended roadmap activities is shown in Appendix B.

An integrated, cross-disciplinary approach is essential to rapid progress. As work group members pondered and debated the gaps in understanding of processes and properties; the shortcomings of existing measurement devices, techniques, and systems; or the inadequacy of process models and integrated site models as predictive simulation tools, a common theme emerged. To make progress and overcome identifiable limitations, it would be necessary to integrate geological, hydrologic, chemical, and biological perspectives, research and testing methods, tools, and data. Creating and working within this ***geological-hydrologic-chemical-biological (GHCB) framework*** emerged as a fundamental change from the discipline-specific approaches that have prevailed in past vadose zone research.

2.0 PHYSICAL, CHEMICAL, AND BIOLOGICAL ASPECTS OF VADOSE ZONE FLOW AND TRANSPORT

Advances in understanding fluid flow and contaminant transport and transformation processes in the vadose zone are closely connected with advances in characterizing and measuring subsurface properties and processes. Advances in both understanding and characterizing/measuring the subsurface system often follow from advances in numerical modeling and computational capability. In turn, the conceptual models on which numerical modeling is based depend on understanding the subsurface properties and processes. And each simulation run depends on data, derived from measurement and characterization, which the numerical models require as input.

To this interdependence among theory (understanding), characterization and measurement (factual description), and prediction/integration (numerical modeling) as aspects of one interlocking scientific process must be added the multidisciplinary character of what is to be understood, described, monitored, and modeled. As noted in the Introduction, the processes that occur in the vadose zone do not respect the traditional disciplinary divisions between geology, hydrology, soil science, chemistry, and biology. Scientists still tend to think in terms of a "coupling," within a geologic setting, of physical (i.e., hydrogeologic) processes, a chemical transformation, and biological activity. In fact, there is just one integrated GHCB system. Investigators trained in one or another specific discipline initially focused on limited aspects of that system to begin understanding it. However, to understand the entire system, and to simulate it realistically enough to produce reliable predictions, an integrated GHCB perspective must be used.

These interdependencies across research methods and disciplines mean that any attempt to set priorities for work in one area soon runs into the work priorities in other areas on which it depends. For the purpose of presentation, some initial separations must be made, although the necessary interconnections must eventually be added. This section covers research needs by basic disciplines. Section 3 outlines the research needed to address the combinations of geological, hydrologic, chemical, and biological aspects found in real vadose zone processes.

This section begins with a context-setting discussion of flow and transport processes in the vadose zone, followed by a brief look at the basic activities required to begin assembling a GHCB framework. (The GHCB framework will be taken up again in Section 4, where it is presented as an interdisciplinary infrastructure requirement.) The next three subsections present research needed to understand, measure, and model the basic physical, chemical, and biological processes and properties of vadose zone systems. The section ends with research needed on three special topics crucial to understanding flow and transport in the vadose zone. These are colloidal formation and transport, multiphase flow and transport, and unstable processes. Within each subsection, activities needed to *understand and model the basic processe*s are presented first, followed by activities required to *possess adequate data and monitoring capabilities*.

As noted above, these areas of research are interdependent. Mid-term and long-term progress in understanding and modeling a process often depends on near-term advances in characterization and monitoring techniques and technology, and vice-versa.

In the sections on measuring and monitoring basic processes, the intent is not to produce a comprehensive review of existing methods. Rather, the intent is to map the science and technology required to advance the existing methods and develop new ones. For a review of existing methods to measure and monitor existing process, the characterization and monitoring work group selected several key review papers and handbooks (Scanlon et al., 1997; Ward, 1990; Wilson, 1982, 1983; Wilson et al., 1995).

2.1 The Importance of a Geological, Hydrologic, Chemical, and Biological Framework

A significant number of subsurface environmental problems involve fluid flow and solute transport in the vadose zone. A key component in assessing contamination hazards and designing remedial actions is the development of flow and transport models. These models are developed to work within a specific physical framework that accounts for appropriate processes at the appropriate scale. The physical framework must include all the relevant geological, hydrologic, chemical, and biological parameters and processes in three-dimensional space, while taking into account changes in these processes and parameters over time and space. These relationships between the geologic, hydrologic, chemical, and biological parameters and the processes linking them constitute the GHCB framework, as that term is used in this report.

Geologic processes of deposition and diagenesis have resulted in highly variable subsurface environments at the priority sites of subsurface contamination across the nation, including those in the DOE complex. The established view is that the hydrologic parameters governing the magnitude and direction of water and vapor flow in these environments are related to a combination of geological structure and post-depositional processes, as is the spatial distribution of mineralogical features. The presence of water and the distribution of dissolved contaminants and nutrients depend on this spatial distribution, in combination with external driving forces (e.g., precipitation).

In vadose zone environments, geological, hydrologic, chemical, and biological properties and processes depend on the system state. The energy of water in contact with the porous medium depends on the moisture content. The geochemical and biologic environment is a function of the water distribution and the geologic character of the medium, and the hydraulic conductivity is a function of moisture content. It is also true that the system state at any given time and place is a function of the physical, chemical, and biological processes that have occurred up to that time.

The properties and processes discussed in the remainder of Section 2 constitute a partial list of state variables and system parameters used to describe flow, transport, and transformation processes in the vadose zone. In general, however, the state variables (e.g., moisture content, pressure head, temperature, and contaminant concentrations) or fluid and medium properties (hydraulic conductivity and solid phase mineralogical or exchange properties) needed to characterize the system state fully in space and time cannot be easily determined by either direct *in situ* or other means. Often, they must be inferred from indirect measurements. Where these state variables or properties can be obtained directly, the measurements are representative of a wide range of support volumes, and are typically collected at various network scales. Obtaining representative values for processes and properties poses an extreme challenge, as does developing relationships for interpolating between measured and inferred properties or parameters.

The long term goal in building a GHCB framework is to develop a quantitative relationship between the geologic nature of a specific site and the parameters and processes that affect contaminant fate and transport at that site. Developing quantitative GHCB models is necessary for numerical simulations, which are used to understand the relationships between parameters and processes. These simulations of a specific vadose zone environment ***as a system*** will ultimately be used for predicting future evolution of the system, as well as understanding its past and current states.

The critical element of infrastructure for developing and making available the multidisciplinary data to support a GHCB framework is referenced here as a GHCB *virtual library*. The activities to develop and make accessible a GHCB virtual library are described in Section 4.1.1. However, Sections 2 and 3 can be viewed as providing an in-depth analysis of the work required to provide the understanding, the data, and the interpretive and predictive tools to populate a GHCB framework for sites with vadose zone contamination.[13]

2.2 Physical Description of Flow and Transport Processes

2.2.1 Understanding Basic Physical Properties and Processes

Our current ability to understand contaminant transport in the vadose zone, predict fluid flow and contaminant transport processes, and manage those processes optimally is limited. For example, we lack adequate understanding of many fundamental interactions between the solid, liquid, and gaseous phases in contaminated subsurface media. Equally or more important, methodologies are lacking to represent flow and transport processes and parameters across different spatial and temporal scales. The necessity for understanding scale differences is a consequence of the overwhelming heterogeneity of the hydraulic and transport properties of the subsurface. Macroscopic continuum approaches that work well for representing flow and transport processes at relatively large spatial scales in homogeneous media may critically misrepresent processes at smaller scales in highly heterogeneous granular or fractured porous media.

Activity PH1. Assess the importance of fluid flow and chemical transport processes and subsurface properties relevant to site characterization, remediation, and long-term stewardship.

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[13] Appendix B contains a complete list of all the S&T roadmap activities presented in Sections 2 through 4.

- **Near-Term Status Point.** Subsurface properties (e.g., gravitational, pressure, temperature, and chemical gradients) of importance to fluid flow and chemical transport at contaminated vadose zone sites have been identified and assessed.

There are many obstacles to describing fluid flow and solute transport more realistically and implementing these process descriptions in predictive models. Improved descriptions are needed for many pore-scale processes and associated liquid-solid and liquid-gas interactions. Driving forces that affect flow and transport (especially chemical gradients) need to be studied. Also needed are more general constitutive relationships among fluid, geochemical, and solid phase parameters and variables. For example, more general representations are needed of two-phase air-water hydraulic properties in unsaturated media under extremely dry conditions.

Activity PH2. Design and conduct laboratory and field experiments to resolve critical gaps in understanding fluid flow and chemical transport processes in granular media. The criticalness of gaps is to be assessed by relevance to environmental restoration and long-term stewardship missions of the DOE and other agencies.

- **Near-Term Status Point.** Critical gaps that can be answered within a decade through laboratory and controlled field experiments have been identified and prioritized.
- **Task Beginning Near-Term with Mid-Term Endpoint.** Design, implement, and analyze results of laboratory and field experiments for the prioritized critical gaps.

Improved process-based descriptions of flow and transport in macroporous soils and unsaturated fractured media represent an especially significant challenge. More realistic representations are needed of the pore-space geometry of such structured media. Emerging geological, pedologic, and topological characterization techniques could be used to develop these representations. In parallel with this effort, improved descriptions of matrix-fracture interactions of structured media must be developed.

Activity PH3. Improve process-based understanding and models for flow and transport in macroporous soils and unsaturated fractured rocks.

- **Task with Mid-Term Endpoint.** Develop realistic representations of pore-space geometry of, and fluid flow in, structured media using geological, pedologic, and topological characterization techniques.
- **Task with Mid-Term Endpoint.** Develop and implement improved descriptions of matrix-fracture interactions.
- **Task with Mid-Term Endpoint.** Develop general constitutive relationships for both granular and structured media.
- **Task with Mid-Term Endpoint.** Develop pore network and other models based upon appropriate equations (e.g. Navier-Stokes), and devise methods for upscaling processes and/or properties from sample to formation scales.

- **Task with Long-Term Endpoint.** Incorporate solid surface heterogeneity (pore and sample scale) with detailed hydrodynamics into solute transport models (to model opportunity times for reactions, streaming potentials, and other processes or variables).

The propagation of physical processes across scales and the associated prediction of uncertainty affects all modeling activities in earth systems. Not only is it necessary to match the proper model to the scale of interest, useful simulation tools must be able to move from one scale to another without losing key elements of the basic processes involved. A related challenge is to both recognize and incorporate significant data at different scales within a robust conceptual model of key flow and transport processes operating at the different scales relevant to site remediation, containment, and long-term stewardship decisions. Meeting this challenge will require methods for efficient assimilation of different types of data having different spatial and temporal resolutions, different geostatistical properties, and different measurement errors.

It is important to recognize the need for proper data at a range of scales. Applying models to real-world situations will require hypotheses about the main processes operative at individual sites and estimates of site-specific properties. These processes and parameters include: (1) hydraulic and solute transport parameters such as capillary-pressure saturation curves, conductivities of liquids and gases as a function of phase saturation; and various diffusion coefficients, tortuosities, and dispersivities; (2) fluid properties such as density, viscosity, enthalpy, vapor pressure, surface tension, and wetting angle; (3) thermal properties such as heat capacities and the saturation dependent bulk thermal conductivity; (4) biogeochemical parameters such as thermodynamic and kinetic data for homogeneous and heterogeneous reactions involving aqueous and gaseous species, minerals, and mineral surface areas; (5) initial and boundary conditions for fluxes, temperature, pressures, fluid compositions, aqueous and gas phase compositions, and mineral concentrations; and (6) fluid and chemical sources and sinks.

Activity PH4. Develop methods for modeling scale-dependent properties and processes and for assimilating data from different scales into these models.

- **Task with Near-Term Endpoint.** Develop and implement improved models for evapotranspiration and root water uptake as a function of water stress and other factors.
- **Task with Near-Term Endpoint.** Develop process-hierarchical approaches for describing and modeling controlling processes (e.g., models of increased complexity for flow in structured media, or increasingly sophisticated process-based approximations for gaseous transport or the flow of non-aqueous phase liquids).
- **Near-Term Status Point.** Methods have been developed to quantify spatial variability in flow and transport parameters, fluid properties, thermal properties, and biological and chemical reactions.

- **Task with Mid-Term Endpoint.** Investigate potential of collecting/inverting multi-scaled data to provide information about variability as a function of scale.
- **Task with Mid-Term Endpoint.** To understand how different measurement methods scale from one level of support to another, experiment with modifying the acquisition parameters for a certain type of method to sample different scales of variability.
- **Mid-Term Status Point.** Methods have been developed for measuring physical processes and properties and their uncertainties across different scales. The multi-scale data from these methods can be assimilated into process models in which the properties and processes can be propagated (in simulations) as, for example, governing equations, driving forces, and/or media properties.
- **Mid-Term Status Point.** Linkages between relevant small-scale processes and properties with larger-scale flow and transport behavior have been identified for cases where no simple upscaling is possible.
- **Long-Term Status Point.** Microbiology modules are incorporated into physical models of solid-gas-liquid environments.
- **Long-Term Status Point.** Solid surface evolution due to biogeochemical reactions (precipitation-dissolution, reduction-oxidation, and other reactions that can change solid-phase geometry and density of exchange sites) has been incorporated into transport models necessary for long time-scale simulations.
- **Long-Term Status Point** (also a status point for Activity PH3). Models for unsaturated flow and transport in different types of porous media have been developed that are both process-adaptive and scale-adaptive. These models invoke the appropriate processes at the appropriate scale and employ the corresponding transport and hydraulic properties.

Our knowledge of basic vadose zone flow and transport processes has advanced considerably over the past several decades. This progress is reflected in the many thousands of papers being published on vadose zone processes annually in dozens of scientific journals. Unfortunately, much of this knowledge is not being used to advantage in the management practices for remediation and stewardship currently being used by many federal agencies, including DOE. In the near term, the nation's capabilities to solve problems involving contamination of the vadose zone and groundwater can be significantly enhanced by narrowing this gap between the state of the art and the state of practice. For this reason, known models and solutions need to be assessed for adequacy in representing flow, geochemical, and microbial transformation processes relevant to site characterization and environmental remediation and stewardship. Critical gaps need to be identified and resolved to further the understanding of these processes, focusing on issues most relevant to the protection of irreplaceable soil and water resources.

Activity PH5. Improve the state of practice in flow and transport models used by government agencies for vadose zone contamination simulations, beginning with DOE.

- **Near-Term Status Point.** DOE flow and transport prediction models and solutions have been updated by incorporating known models/modules with a more sound physical-chemical basis.
- **Task with Mid-Term Endpoint**. Integrate critical elements of chemistry and microbial activity in models for liquid flow and solute transport.

2.2.2 Measuring Physical Properties and Processes

Characterization and monitoring of flow and transport properties and processes in the vadose zone includes measurement of state variables such as moisture content, soil water potential, and temperature, and the description of flow and transportation in disturbed and undisturbed media. Flow and transport description includes measuring hydrologic parameters such as permeability and porosity as a function of time and space, the flow architecture including fractures, and the suite of methods (e.g., tracers) used to map the subsurface.

2.2.2.1 Moisture Content, Matric Potential, and Temperature

Methods for assessing hydrologic state variables are primarily invasive and have not evolved much in several decades. Key areas for development include improving robustness; easing emplacement costs and containment system concerns; and simplifying data communication, fidelity, and manpower requirements.

Among the most important state variables requiring characterization in the vadose zone are water content, matric (soil water) potential, and soil temperature.

- **Water content**, the mass of water held in a porous medium, is often reported as percent saturation. Water content measured on a volumetric basis (volume of water per volume of voids) is needed to make predictions of contaminant transport through the vadose zone and for mass balance calculations.
- **Matric potential** is the energy status of water in soil or other material resulting from its presence in the gravitational force field, capillary and surface forces, and from the presence of mineral salts. Soil water potentials are needed to determine gradients for water flow.
- **Soil temperature** affects many processes such as microbial activity, water and vapor movement, and geochemical reactions.

Activity PH6. Develop, improve, and confirm methods for measuring basic hydrologic properties.

- **Near-Term Status Point.** Moisture content, matric potential, and temperature measurements are no longer a major source of uncertainty for site-wide monitoring and modeling. Monitoring approaches for these properties are robust enough to cover long-term stewardship responsibilities.

2.2.2.2 Distribution of Flow and Migration (Perturbed and Unperturbed)

Mapping water distribution and tracking water migration in the vadose zone are among the most important tasks for noninvasive monitoring. Tracking water movement may reveal fundamental formation parameters such as porosity and permeability.

At present, water saturation within the vadose zone is poorly determined from geophysical measurement; time-lapse studies of water movement have done better. Both electrical and seismic techniques typically have good sensitivity to water saturation in the vadose zone, but there are many other competing factors that make isolating the effects of water saturation difficult. This suggests that research should be focused on approaches using several independent measurements. Other promising technologies include spectral induced polarization, borehole radar or ground penetrating radar, spectral inductive electromagnetic measurements, and microgravity measurement.

The ultimate research goal is to provide capability to map water distribution and track flow within a volume of interest in an arbitrary geology, using cost-effective noninvasive technology. The status points listed below for this research activity represent increments of progress toward this goal. Achieving the long-term status point will require both an improved imaging technology and better integration with hydrologic and geological information.

Activity PH7. Improve the capability to track subsurface fluid flows with increased precision, over larger areas, and at greater depths underground.

- **Near-Term Status Point.** Improved resolution and decreased uncertainty. Example, fluid movement (such as in an infiltration event) in a 10 m X 10 m area, at depths up to 100 m, can be tracked to a precision of 10 percent.
- **Mid-Term Status Point.** Further improvements in resolution and uncertainty reduction. Example: fluid movement in a 50 m X 50 m area, at depths up to 100 m, can be tracked to a precision of 5 percent.
- **Long-Term Status Point.** Greatly improved resolution and reduced uncertainty. Example: a three-dimensional pulse of water (2 m X 2 m) can be identified to a precision of 2 percent at depths up to 100 m.

2.2.2.3 Using Tracers (Natural and Introduced) to Determine Flow and Transport

Characterization and modeling of subsurface flow and transport is critical for evaluating the current distribution of subsurface contaminants and predicting future migration. Natural and anthropogenic tracers can be used to determine directions and rates of transport, assess flow processes, and validate numerical models.

The subsurface distribution of contaminants can be thought of as a large-scale applied tracer experiment. However, it is often difficult to reconstruct the location and timing of contaminant releases. The research challenge is to provide a consistent system model that optimizes the use of tracers, extracting as much information about the subsurface as possible while providing data to complement information from other approaches.

Activity PH8. Optimize the use of natural and anthropogenic tracers for determining directions and rates of transport, assessing flow processes, and validating numerical models.

- **Task with Long-Term Endpoint.** Develop, test, and confirm the inverse process of using tracers to estimate fluxes and ages of pore water. Include methods to propagate uncertainties in tracer measurements to obtain uncertainties in calculated fluxes and ages.
- **Long-Term Status Point.** A variety of tracers are available for use in locating contaminants, establishing the role of surface boundary conditions in specific subsurface environments, and obtaining point estimates of fluxes and ages.

2.2.2.4 Quantification of Flow in Fractures

Rock fractures and soil micropores often serve as preferred pathways for migration of contaminants. In unsaturated fractured rock, fractures almost always represent zones of permeability that are different from normal, unbroken rock (e.g., tuffs, basalts, and granites) or undisturbed materials (e.g., alluvia and colluvia). Consequently, the physical properties of fractures must be known, to evaluate flow regimes, perform modeling calculations, and plan remediation where fractured rock strata are present in the vadose zone.

The spatial distribution, trace length, and connectivity distribution of fractures are often inferred using cores, outcrop data, hydraulic tests, seismic and electromagnetic surveys, borehole logging tools including borehole cameras, temperature logs, and flow meters (Long and Witherspoon, 1985; Paillet, 1997). Such efforts to characterize fractures are largely used to understand and model groundwater flow. Major exceptions are the work to characterize fracture networks within the vadose zone at the Yucca Mountain Project in Nevada and the Apache Leap site in Arizona.

Flow in Fractures. For both groundwater and vadose applications, a key challenge is to capture the spatial variations of the fractures or fracture systems efficiently, regardless of local borehole stress conditions. A crucial criterion for successful fracture characterization is distinguishing between the presence of any or all fractures and the subset of fractures that serve as conduits or barriers for fluid migration. Another key challenge is to identify actual flow in fractures and in turn identify contaminants in the fluid flowing within the fractures. These goals for long term research represent a significant challenge because little remote sensing research, either in-situ or in the subsurface, has been done on flow detection and flow characterization within fractures.

The ability to detect and determine the nature of fluid in fractures from surface or borehole measurements is important in many geological environments, but especially so in hard rock. In hard rock environments, fluid contaminants are stored and migrate principally in the fracture network. Currently no surface methods can reliably detect fluid in fractures in the vadose zone. There have been reported successes of crosshole radar measurements detecting injected tracer fluid in fractures, but there are no cases where *in situ* fluid in fractures has been detected or imaged. The best candidate technologies appear to be seismic techniques and radar, which provide both the required range and resolution. Other interesting possibilities include geochemical methods, electrical and electromagnetic techniques, and logging techniques. The goal is to detect the presence of fluid in fractures and to quantify the amount in real time from the surface.

Geophysics Focused on Fractures. Crosshole geophysical data are currently used to determine whether fractures are present, as well as to identify water-conducting fracture pathways. Crosshole geophysical techniques may also provide information about the presence and nature of fractures away from the borehole wall. Surface geophysical techniques include the use of P-wave reflection to detect shallow faults with offsets as small as two or three meters. A potentially useful seismic method is diffraction enhancement; research on relatively high frequency (10–100 Hz) surface waves in multi-channel analysis of surface waves suggest that faults and joints might be routinely detectable with surface waves. Other general issues related to geophysical fracture characterization include fracture imaging and sensor development, understanding geophysical responses to fractures, and integrating interpretations to address scaling.

Activity PH9. Develop capability to detect the presence and movement of fluid in fractures and fracture networks.

- **Near-Term Status Point.** The presence of fluid in individual fractures can be detected in some cases.
- **Task with Near-Term Endpoint.** Quantify the relationships among the most likely geophysical methods or combinations of methods that will provide fracture diagnostics.
- **Mid-Term Status Point.** Contaminant fluid in fractures can be detected in most cases.
- **Task with Mid-Term Endpoint.** Discover and quantify new relationships between surface geophysical measurements and fractures, so that fractures a few centimeters across at depths of 10 meters can be routinely mapped.
- **Long-Term Status Point.** Contaminant fluid in fractures in real time can be detected and quantified from the surface or in boreholes.
- **Long-Term Status Point.** Low-cost, automated, and reliable geophysical techniques are available for mapping fractures immediately at the field site, without delays for processing or analysis.

2.2.3 Integration of Geophysical and Hydrologic Data

Many of the problems and initial costs of subsurface remediation come from field site characterization. Three-dimensional information about the heterogeneous subsurface is needed in order to identify the key controls on flow and contaminant transport processes. It is widely recognized that natural heterogeneity and the large spatial variability of permeability predominantly control the flow field, and hence transport. Moreover, natural heterogeneity exhibits variability over a wide range of scales and is difficult to characterize using only one-dimensional borehole data.

Geophysical data can complement direct borehole characterization data by providing multidimensional subsurface measurements in a minimally invasive manner. Crosshole methods have the potential to provide high-resolution information about geophysical attributes in the intra-wellbore area. A goal for environmental characterization should be to use these high-resolution, multidimensional images of geophysical attributes to infer key hydrologic properties of the subsurface.

However, several obstacles remain to be overcome before crosshole tomographic data can be used routinely and reliably for estimating hydrologic properties. Some of the issues are briefly described below, under the topics of petrophysical relationships, estimation methodologies, and inversion approaches. Roadmap activities to address these three topics are listed immediately afterward. The important issue of scaling, as it applies to interpretation of geophysical data and integration with other GHCB data, is discussed more fully in Section 3.2, which covers roadmap activities relevant to scaling.

2.2.3.1 Petrophysical Relationships

The relationships between measurable geophysical attributes of a body of rock and its hydrologic parameters such as porosity and water content are called *petrophysical relationships*. Much work has been dedicated to investigating such relationships for consolidated rocks at higher pressures (greater than 15 Mpa, conditions common for petroleum reservoirs). However, research on petrophysical relationships for near-surface sites is still in its infancy. Currently, most investigations obtain, at best, a site-specific relationship between co-located geophysical attributes and hydrologic parameters. Few attempts have been made to move beyond site-specific characterization of these relationships to fully understand the interaction between field-scale geophysical responses and the physical properties of the medium.

Similarly, there has been little research on how to include data on multiple geophysical attributes in the petrophysical relationship, in order to reduce uncertainties. Nor has there been much research on resolving the non-uniqueness conditions that are sometimes inherent in petrophysical relationships.

2.2.3.2 Estimation Methodologies

Routine procedures must be developed to integrate geophysical tomographic data rigorously with existing direct measurements from wellbores and with other data (geological information, surface geophysical data, chemical data, and biological data). These integration methods also must provide better estimates of uncertainty arising from measurement error, inversion error, and use of an estimated petrophysical relationship. We must understand how to use multiple, co-located data sets to reduce the ambiguity and uncertainty associated with parameter estimates. Stochastic methodologies have been developed to handle some of these issues, but the methodologies would benefit from refinement and further testing and extension with scale issues in mind. (These and other issues in estimating and reducing uncertainty are discussed further in Section 3.3, along with roadmap activities specifically addressing uncertainty.)

2.2.3.3 Inversion Approaches

Inversion approaches, such as those involving crosshole tomography, must be further developed and tested. Consensus must be reached on appropriate data correction procedures prior to inversion. More advanced approaches such as constrained inversion, stochastic inversion, and joint geophysical-geophysical or geophysical-hydrologic inversions need further investigation, including testing and validation. We should investigate how to weigh the information content of the different geophysical data prior to joint inversion, how to invert data having different resolutions, and how to provide uncertainty estimates that correspond correctly to the inverted tomographic attributes.

To translate geophysical attributes into hydrologic parameters, issues of scale must be considered. The large spatial variability of hydraulic properties in natural geological systems over a wide range of scales increases the difficulty of estimating hydraulic parameters and their spatial correlations from geophysical attributes and imagery. Further, the obtained measurement value is a function of the subsurface volume interrogated by the instrument (sometimes called the instrument support scale), as well as the network scale (acquisition parameters/instrument spacing), compounding the problem. Both the instrument and network scales vary among and even within geophysical methods. Thus, it is crucial to understand how these measurement-related scales impact obtained values and how to incorporate different types of measurements with each other. A general understanding is needed for how to scale measurements collected in the laboratory for use in the field, how to use petrophysical relationships developed in the laboratory with field data, and how to integrate different geophysical data that sample different volumes.

Activity PH10. Characterize the petrophysical relationships for translating geophysical attributes in near-surface strata into estimates of hydrologic parameters relevant to vadose zone contamination (e.g., porosity and water content).

- **Near-Term Status Point.** Generalized petrophysical relationships between geophysical attributes and hydrologic parameters have been developed for near-surface environments.
- **Task with Near-Term Endpoint.** Investigate how multiple types of geophysical and other data reduce uncertainty in applying petrophysical

relationships and can aid in resolving issues of non-uniqueness in relationships between geophysical and hydrologic parameters.

- **Mid-Term Status Point**. The mechanisms of geophysical energy propagation at the field tomographic scale within unconsolidated or loosely consolidated, low pressure, granular porous material are understood.
- **Mid-Term Status Point.** Joint and constrained inversions that honor all data can be performed. How additional data improve the estimate and decrease the estimation error is understood. Data with different measurement scales can be incorporated in the inversion process correctly.
- **Task with Mid-Term Endpoint.** Develop a quick and reliable way to assess the extent of a vadose zone contamination problem relative to the scale of the hydrologic heterogeneity so that the most appropriate techniques and acquisition parameters can be selected for characterizing the key parameters that control flow and transport at that site.
- **Long-Term Status Point.** Methods to scale between laboratory-scale and field-scale measurements are known and in use. A variety of differently scaled data can be reliably incorporated into geophysical inversions to provide an integrated and hierarchical interpretation of hydrologic properties.

Activity PH11. Improve and apply geophysical methods for characterizing near-surface environments typical of sites with vadose zone contamination.

- **Task with Near-Term Endpoint.** Develop automatic data picking and quality control approaches for crosshole tomographic methods.
- **Task with Near-Term Endpoint.** Investigate the utility of constrained and joint inversion for improved estimation of hydrologic parameters. Develop stochastic inversion procedures that yield distributions of possible geophysical attributes at each location.
- **Near-Term Status Point.** Stochastic estimation techniques that provide an estimate of the property of interest, as well as information about its uncertainty, have been tested and applied to contaminated vadose zone sites.
- **Near-Term Status Point.** Incorporate measurement support scale, and other means of recognizing the importance of scale, when applying geophysical methods to estimate hydrologic properties and correlation lengths.
- **Mid-Term Status Point.** Hydrologic properties (e.g. water content, permeability and porosity) and their associated uncertainties and spatial correlation functions are being estimated from different types of geophysical data such as crosshole tomographic imagery. These estimates are conditioned to direct measurements, with attention to scale, using hierarchical spatial scale estimation procedures with multi-scaled data.

Long-Term Status Point (applies to Activities PH10 and PH11). Practical guidelines for different environments allow quick field tests to determine the characterization regime into which the vadose zone at a contaminated site falls. The governing petrophysical relationship for that regime is used to interpret the geophysical data to obtain first-pass estimates of key flow and transport parameters.

Long-Term Status Point (applies to Activities PH10 and PH11). Tomographic methods can supply real-time, multidimensional (spatial and temporal), automatic interpretations of hydrologic properties or changes in properties due to bacterial modification, environmental remediation, infiltration, and other dynamic processes. The fully automated inversion process may also incorporate varying scales, but must provide real-time estimates of hydrologic properties at high resolution.

2.2.4 Highlights of Roadmap Results for Physical Description of Flow and Transport

Table 1 highlights some of the major results that can be anticipated from these 11 research activities addressing physical processes and properties. The time horizons indicated in the table are contingent on sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under the activities.

Table 1 Highlights of Results for Physical Description of Flow & Transport Research Activities

	Near Term	Mid Term	Long Term
Computer models used by federal agencies and others incorporate the best state-of-the-art conceptual models and implementations (software modules).	◆		
We can detect the presence of fluid in fractures in some cases.	◆		
We can distinguish, in most cases, the subset of fractures that are conduits for fluid flow and contaminant transport.		◆	
We can map and predict water distribution and flow through structured soils or fractured rock at multiple spatial scales.		◆	
Monitoring data on fluid flow and contaminant transport can be interpreted and represented visually at site-wide scales in real-time.			◆

2.3 *Chemical Properties and Processes*

The roadmap pathways for chemical properties and processes divide into two broad categories: 1) understanding reactive flow and transport, and 2) measuring and modeling chemical properties and processes in the vadose zone environment.

2.3.1 Understanding and Modeling Basic Chemical Properties and Processes

Numerical continuum models of reactive flow and transport in heterogeneous, variably saturated, nonisothermal porous media have advanced considerably in the past several years. It is now practical to carry out simulations in one or two spatial dimensions, on small to medium sized grids (2,500-10,000 nodes), for coupled, transient, flow and transport that is both ***multiphase*** (aqueous, gaseous, CO_2, and non-aqueous phase liquid (NAPL)) and ***multicomponent*** (on the order of 10-20 degrees of freedom). Processes that can now be incorporated in these simulations include:

- Homogeneous reactions involving aqueous complexing, ion pairing, and redox reactions,
- Heterogeneous reactions consisting of mineral precipitation and dissolution, sorption, and aqueous-gaseous reactions, and
- Transport and reaction with colloids.

Reaction rates may be described either through kinetic rate laws or local equilibrium, as appropriate. In addition, flow and transport may be sequentially coupled, thus accounting for changes in porosity and permeability resulting from chemical reactions.

Few, if any, computer codes currently account for all of these different features. Although limited work has begun on developing next-generation codes for three-dimensional simulations with large numbers of unknowns, to be run on massively parallel computing architectures, development of optimally efficient and powerful parallel algorithms is still in its infancy.

Continuum models that incorporate various levels of geochemical complexity do exist. However, key research challenges are to parameterize these codes, develop more accurate rate laws, and understand the relationships between chemical and physical changes occurring in porous media. Roadmap activities for these research areas are discussed below.

2.3.1.1 Parameterization of Codes

Computer codes for geochemical reactive transport require representations of key chemical parameters, such as the characteristics of contaminated solutions that determine the rates at which they react with their local geochemical environment. Algorithms and databases exist for modeling aqueous solution chemistry at 25°C and ionic strengths less than approximately 1 molar, using extended Debye-Hückel coefficients to correct the chemical activities. For higher temperatures and high ionic strengths, however, the thermodynamic data are sparse. Although measuring these properties requires stringent laboratory conditions, existing technologies are adequate to obtain the needed data.

Activity CH1. Extend solution chemistry models to higher temperatures and ionic strengths (e.g., Pitzer equations) relevant to vadose zone contamination problems.

- **Near-Term Status Point.** Solution chemistry models have been extended to temperatures and ionic strengths needed for most vadose zone contamination problems, including DOE contamination sites.

2.3.1.2 Accurate Rate Laws

Rate laws used in existing computer codes are commonly based on transition state theory or simple reaction kinetics. Rate constants for kinetic descriptions of mineral reactions have been obtained over a limited temperature range and for limited compositional variables, primarily pH. Often, however, rate laws measured in the laboratory are not suitable for direct use in a reactive transport model because they do not cover a suitable range of conditions. For example, the oxidation state of the system may change from oxidizing to reducing along the flow path. Rate laws are needed which encompass the variation in oxidation state and other conditions over the entire flow path.

Mineral rate laws apply to crystalline phases and not to glasses or phases with mixed structural states, such as mixed-layer clays. Rate constants for relevant homogeneous redox reactions are largely unknown. Subsurface low-temperature systems are often in redox disequilibrium. The reaction kinetics for these systems is also strongly coupled to the available reactive surface areas of potential reactant phases. Finally, nucleation mechanisms are often poorly understood, thus preventing adequate description of conditions leading to supersaturation, which results in inappropriate kinetic descriptions of the processes involved.

While ion exchange and surface complexation models are commonly used in reactive transport models, the data needed to support these models are generally not available. Furthermore, the available data are limited primarily to 25°C for conditions of local chemical equilibrium. These conditions are not typical of contaminated near-surface vadose zone environments. Surface complexation models also often fail to conserve charge when combined with transport processes.

Activity CH2. Improve the understanding of kinetic rate mechanisms and effective surface areas, in order to develop improved rate laws.

- **Near-Term Status Point.** Reaction kinetics and rate laws have been formulated that are appropriate for use in numerical continuum models of reactive flow and transport for many vadose zone contamination problems, including DOE sites.
- **Long-Term Status Point.** Databases of appropriate reaction rate constants applicable to refined reaction rate laws have been developed through experimental studies.

2.3.1.3 Linkages between Chemical and Physical Changes in Porous Media

Chemical reactions sometimes alter the physical properties of the medium. Reactions of primary importance are mineral precipitation and dissolution and biomass formation and destruction. Such changes are difficult to quantify and usually require phenomenological formulations based on experiments. Typical coupled processes include changes in porosity and permeability, surface armoring, and changes in cation exchange capacity and surface site density.

Activity CH3. Investigate cation exchange capacity and surface site density/complexation reactions on mineral surfaces and colloids for systems typical of vadose zone environments and contamination problems. Resolve the importance of lack of charge conservation in surface complexation models when combined with transport, possibly by including streaming potentials in the formulation.

- **Task with Near-Term Endpoint.** Determine if significant differences exist for measurement of cation exchange capacity and surface site density between *in situ* field measurements of undisturbed samples and laboratory batch measurements involving disturbed media. Validate conditions under which batch K_d measurements can be used to estimate retardation in variably saturated flowing systems.
- **Mid-Term Status Point.** The kinetics (including reversibility) of ion exchange and surface complexation reactions on mineral surfaces and colloids has been determined for most solution-solid systems relevant to vadose zone contamination problems.

Activity CH4. Investigate the effects of dissolution and precipitation on porosity, pore structure, and permeability. Study nucleation controls that may bias dissolution and/or precipitation to particular pore environments.

- **Task with Mid-Term Endpoint.** Develop a functional description for porosity/permeability evolution reflecting chemical effects.
- **Task with Mid-Term Endpoint.** Develop rate laws for glass dissolution and solid solutions that cover more extended conditions typical of natural and contaminant-affected flow fields. Improve models of nucleation processes.

Long-Term Status Point (applies to Activities CH1 through CH4). Kinetics and rate laws have been formulated for ion exchange and surface complexation processes coupled with mineral precipitation and dissolution. This knowledge has been validated in field experiments and incorporated in reactive flow and transport models for vadose zone systems.

Porous media in the unsaturated zone typically contain gaseous, solid, and liquid phases in which phase boundaries can significantly alter the geochemistry of both indigenous minerals and contaminant species, as well as liquid phase properties. The effects can be especially important in very dry situations involving low water contents and thin liquid films covering the solid phase.

Activity CH5. Investigate phase boundary conditions occurring in vadose zone environments that may significantly influence liquid flow and contaminant transport.

- **Task with Mid-Term Endpoint.** Develop accurate models for mineral reactions in contact with a thin liquid film that may have different properties compared to bulk fluid (e.g., for extreme evaporation conditions that may favor formation of evaporite mineral phases).

- **Task with Mid-Term Endpoint.** Develop accurate models for mineral reactions in unsaturated systems having variable gas phase chemistries (e.g., low and high CO_2 or O_2).

2.3.2 Measuring Chemical Properties and Processes

The role of chemical characterization and monitoring in the vadose zone is to describe chemical fate and transport in space and time. From this description, the concentration and extent of contaminants can be determined, and appropriate conceptual models of transport can be developed to aid in prediction and planning.

Assessing accurately the spatial distribution and concentration of contaminants is an essential first step in addressing most problems of environmental contamination faced by problem owners, such as DOE and DOD, or regulators such as EPA. At present, the concentration and extent of contamination is usually determined using invasive sample collection methods (typically boreholes) and laboratory analysis of samples. *In situ* probes can monitor some contaminants with near-real-time analysis and transmit data using datalogger technology. Some contaminants (e.g., radioactive constituents) can be observed using borehole geophysical methods. In most cases, however, concentrations are measured only at a discrete time interval (e.g., quarterly) and only for a limited number of spatial points.

To improve our current methods, five tasks must be accomplished. The first task is to select technologies that can identify the characteristics of individual contaminant species. Candidate technologies include spectral induced polarization; nuclear magnetic resonance; spectral electromagnetic techniques including radar, neutron logging technology; and chemical sniffing methods. Second, researchers must establish the relationship of the measurements to the contaminant species. Through laboratory analysis, chemical species can be isolated by their geophysical or geochemical responses. A third task is to determine the sensitivity limits of the measurement to the contaminant species and their concentrations. Fourth, prototype tools or combinations of tools suitable for a restricted environment need to be deployed. Finally, consideration must be paid to newly invented tools and approaches and other innovations that may be used to improve current methods.

Activity CH6. Improve and develop methods of identifying chemical contaminants in the vadose zone.

- **Near-Term Status Point.** The presence of individual chemical contaminants in soils or other vadose zone strata can be determined from surface or borehole measurements, although field results may require verification with laboratory analyses.

- **Mid-Term Status Point.** Concentrations of the most abundant species (except those at very small concentrations) can be determined within an order of magnitude.
- **Long-Term Status Point.** Contaminated volumes can be isolated, and the concentration of abundant chemical species can be determined to within 10 or 20 percent.
- **Long-Term Status Point.** The volumes and spatial distributions of resident contaminants at or near source discharge points can be quantified for metals, radionuclides, and organics.

2.3.3 Highlights of Roadmap Results for Chemical Properties and Processes

Table 2 highlights some of the major results that can be anticipated from these nine research activities for chemical processes and properties. The time horizons indicated in the table are contingent on sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under the activities.

Table 2 Highlights of Results for Chemical Properties & Processes Research Activities

	Near Term	Mid Term	Long Term
Reaction kinetics and rate laws (in solution) have been formulated for priority vadose zone conditions.	◆		
Individual chemical contaminants in the vadose zone can be detected.	◆		
We understand the kinetics for important chemical reactions at solid and liquid interfaces (e.g., ion exchange and colloids) in vadose zone conditions.		◆	
Flow and transport models map and predict important vadose zone chemical interactions, including those involving mixtures of solids, liquids, and air.			◆

2.4 Biological Properties and Processes

Microorganisms are directly or indirectly responsible for numerous processes that influence the mobility and persistence of contaminants in the vadose zone. They use many organic pollutants as carbon sources or as electron donors or acceptors in biochemical oxidation-reduction reactions. Many metals and radionuclides are metabolically transformed into chemical species that may be either more or less susceptible to long distance migration than their pre-metabolite forms. In addition, microorganisms can have a profound influence on their immediate environment by altering porosity, surface characteristics, pH, or oxidation potentials. These environmental changes in turn affect contaminant transport.

2.4.1 Understanding Biological Properties and Processes

In contrast to the saturated zone, for which a relatively large microbiological knowledge base exists, much less information is available on the distribution, rate, and controls of vadose zone microbial processes. The vadose environment poses a number of challenges to quantifying microbial processes. Concentrations and fluxes of carbon and other nutrients are often very low, and their distributions are heterogeneous. Inputs of nutrients, via rainfall or other means, to the vadose zone at many contaminated sites in arid climates are minimal and intermittent. Infiltration is often localized to fractures and regions of preferential flow. Thus, microorganisms may have to survive long periods of dormancy, yet be prepared to take immediate advantage of transient and often brief influxes of nutrients. As a consequence of these and other constraints, microbial activity tends to be discontinuous and patchy in both time and space.

Transport and colonization of microorganisms is another important issue. Microbes and contaminants are generally not co-located. A major challenge of engineered bioremediation is the delivery of microorganisms to sites of contamination.

Many of the mechanisms for microbial interaction with a few specific contaminants are known. But much remains to be learned about the parameters that control the rate of transformations of radionuclides and mixtures of contaminants, as well as microbial processes in general under extreme conditions. In addition, it is not well understood how the unique hydrologic features of the vadose zone affect metabolism, growth, and microbial transport processes or the distribution of these processes. An understanding of these interactions and processes is required for reliable predictions of contaminant transport (enhanced transport and natural attenuation) and the potential for successful engineered bioremediation.

There are three major research goals to be accomplished:

1. Understand the mechanisms of microbial-contaminant interactions, including biodegradation and transformation, mobilization, complexation, and precipitation, for inorganics and contaminant mixtures in contact with vadose zone materials and engineered biotreatment zones.
2. Conduct field and laboratory experiments and characterization to develop mathematical descriptions of key microbial processes and their linkage to spatially variable hydrogeological and geochemical processes.
3. Apply emerging measurement and sampling technologies for understanding *in situ* rates and scaling of microbial populations/activities in heterogeneous systems to scales relevant for field-scale modeling.

The following four activities address these research goals.

Activity B1. Understanding the mechanisms of microbial-contaminant interactions.

- **Task with Near-Term Endpoint.** Quantify rates of microbial processes affecting inorganics, chelate-inorganic complexes, inorganic complexes, and organic contaminants; identify the factors controlling those rates.
- **Task with Near-Term Endpoint.** Understand and predict how contaminant bioavailability affects, and is affected by, microbial processes.
- **Task with Near-Term Endpoint.** Characterize microbial-mediated corrosion and biodeterioration of materials used to contain contaminants at DOE sites and other sites with contained buried wastes.
- **Task with Mid-Term Endpoint.** Improve the conceptual and mathematical characterization of interactions between microorganisms and contaminants (e.g., biodegradation, immobilization, transformation), microbial and physical/chemical processes (coupled processes), and incorporate these relationships into reactive transport models.
- **Task with Mid-Term Endpoint.** Elucidate pore-scale interactions between microorganisms and contaminants, under undisturbed conditions, including studies: (1) at the microscopic level; (2) at interfaces (solid/liquid, liquid/gas, liquid/liquid, solid/gas, and along textural discontinuities); and (3) in biofilms.
- **Task with Mid-Term Endpoint.** Determine the importance to contaminant transport and preferential flow of microbial attachment/detachment, biofilms, and microbial associations with colloids.

Activity B2. Understand how mixtures of contaminants affect microbial activity with respect to flow and transport of specific contaminants.

- **Mid-Term Status Point.** Conditions under which toxicity of radionuclides, metals, or organics prevent removal of readily degradable organic contaminants have been identified.
- **Mid-Term Status Point.** The rates of biodegradation of particular contaminants can be predicted as a function of the type and concentration of other contaminants present.

Activity B3. Understanding microbial community composition and activity.

- **Near-Term Status Point.** Rapid statistical and classification methods for handling large data sets generated from the characterization of microbial communities have been developed and applied.
- **Mid-Term Status Point.** Microbial diversity in representative vadose zone systems has been characterized (measured), and the factors governing diversity have been determined. Relationships between diversity and community response to contaminants have been determined.

- **Task with Mid-Term Endpoint.** Understand the potential roles of siderophore, surfactant, and chelate production by microbial communities, including the plant root–microbial community interface, on contaminant transformations in engineered biotreatment zones and in contaminated sites without engineered biotreatment.
- **Long-Term Status Point.** The spatial distribution of microbial biomass, activity, and community composition in the vadose zone can be predicted with respect to contaminant distribution. Effects on the microbial distribution from water inputs, contaminant fluxes, and duration of exposure to contaminants can also be predicted.

Activity B4. Characterization methods to understand *in situ* rates and community activities at scales relevant for field-scale modeling.

- **Task with Mid-Term Endpoint.** Characterize microbial transport in different natural porous media and through/from engineered biotreatment zones relevant for vadose zone contamination sites (DOE and others). In particular, characterize transport through unsaturated fine and coarse sands and fractured rock, as a function of water saturation and solution chemistry.
- **Long-Term Status Point.** *In situ* rates of microbial biotransformation of contaminants at contaminated sites can be predicted as a function of site and environmental conditions.
- **Long-Term Status Point.** Information about the composition of vadose zone microbial communities has been incorporated into pollutant fate and transport models.
- **Long-Term Status Point.** Transport of native and introduced microorganisms at contaminated vadose zone sites can be predicted.

2.4.2 Measuring Biological Properties and Processes

Biological processes are important for methods of vadose zone characterization and monitoring in two ways. First, microorganisms are involved in many processes affecting contaminant transport and transformation, and their effects must be quantitatively understood. Second, biological processes, biomolecules, and biomaterials can be used as components in instruments and sensors for characterizing and monitoring the vadose zone.

Non-invasive techniques have been used only in an exploratory fashion to observe the distribution and activity of microbes in the subsurface. Nearly all state-of-the-art microbiological characterization methods currently require invasive sample collection. Most also require subsequent laboratory analysis (rather than incorporating downhole data collection). These requirements result in several problems: high cost, inability to measure rates *in situ*, general lack of joint measurements, and inadequate scale of measurements.

In addition, as noted in the previous section, microbial processes in the vadose zone exhibit spatial heterogeneity and nonlinear temporal dynamics. Small and local variations in physical and chemical properties can result in large differences in subsurface microbial populations and activities. Because invasive sampling and laboratory analysis are required to assess these activities, resolution of spatially heterogeneous and temporally varying microbial distributions is a particularly difficult problem.

Three major types of microbial data are needed for site assessment and site monitoring: bioavailability, *in situ* rates, and community composition and activity. Forged by the intersection of biology, microfluidics, microelectronics, and micro-optics, biotechnological advances pertinent to all three types of data are occurring rapidly in the private sector. However, investments in research are necessary to adapt and apply these advances to vadose zone science and stewardship.

Bioavailability. It is important to know what concentration or mass of a contaminant is immediately available for microbial transformation or is capable of toxic effects on organisms. Ways are also needed to measure the fraction that may eventually become available. Among the potential means to acquire these data are improved *in situ* sensors and development of other approaches.

Activity B5. Developing and improving measurement techniques for bioavailability.

- **Near-Term Status Point.** Improved bioavailability sensors and/or assays have been developed.
- **Mid-Term Status Point.** *In situ* bioavailability sensors have been developed and are in application.

In situ rates. We need approaches for measuring *in situ* rates at scales of intermediate (0.1 to 10 m^3) and miniature (millimeters to centimeters) interrogation volumes. For field applications, approaches using gases and/or solutes are needed, similar to the *in situ* respiration test. (This test measures the rate of depletion of injected oxygen to estimate degradation rates for petroleum hydrocarbons.) Challenges to using these approaches successfully include: (1) development of instrument systems that minimize changes in moisture status and reduce the creation of near-wellbore artifacts during the assay, and (2) sufficient analytical sensitivity for *in situ* processes, which are often very slow.

Activity B6. Developing and applying sensors and sensor systems for *in situ* rate measurements.

- **Near-Term Status Point.** Sensors and systems for *in situ* rate measurements have been developed.
- **Near-Term Status Point.** Chemically reactive contact foils and films for *in situ* rates and/or potential activity have been developed.

Community composition and activity. Rapid advances are occurring in high-resolution signature lipid biomarkers, DNA chips, and other nucleic acid methods for characterizing microbial community structure, diversity, and activity. These measurements are important for improving our understanding of vadose zone microbiological processes and linking communities to functions. However, the per-sample cost is high.

Activity B7. Developing and applying systems for measuring microbial community composition and activity.

- **Near-Term Status Point.** Sample-to-answer analytical systems for community composition and activity have been developed.
- **Near-Term Status Point.** Spectroscopy-based and synchrotron-based inferences of microbial activity have been developed.
- **Task with Near-Term Endpoint.** Perform laboratory studies and develop models of the bio-electric level as a function of different soil types and microbes (aerobic versus anaerobic, a variety of metal-reducing and organics-reducing microbes).
- **Mid-Term Status Point.** Inexpensive sample-to-answer analytical systems for community composition and activity are being applied.
- **Task with Mid-Term Endpoint.** Develop instrumentation to detect lower levels of activity and validate this instrumentation in intermediate-scale and field-scale tests.

Three important long-term status points apply to all three of these roadmap activities for measurement of subsurface microbial communities and activities.

Long-Term Status Point (applies to Activities B5–B7). Economical analysis of spatial distribution and temporal dynamics has been developed and applied.

Long-Term Status Point (applies to Activities B5-B7). Nondestructive joint measurement of biological, geochemical, physical, and hydrologic properties or processes has been extended to intact cores and possibly to the subsurface.

Long-Term Status Point (applies to Activities B5-B7). Proxy measurements for microbiological properties and processes have been developed.

2.4.3 Highlights of Roadmap Results for Biological Properties and Processes

Table 3 highlights some of the major results that can be anticipated from these seven research activities for biological processes and properties. The time horizons indicated in the table are contingent on sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under the activities.

Table 3 Highlights of Results for Biological Properties & Processes Research Activities

	Near Term	Mid Term	Long Term
We understand and can predict how microbial processes affect or are affected by bioavailability of important contaminants.	◆		
We can measure biochemical rates, in situ bioavailability, and the composition and activity of microbiological communities.	◆		
Reactive transport models can predict how microorganisms will interact with contaminants.		◆	
Inexpensive systems are available to measure community composition and activity.		◆	
We can accurately predict site-specific biodegradation rates for important contaminants.			◆
We can take biological measurements along with others without destroying the samples.			◆

2.5 Colloidal Formation and Transport

Many contaminants such as radionuclides and metals are often strongly sorbed by soil and sediments, thus limiting their transport in the subsurface. In some instances, however, strongly sorbing contaminants have been found at locations far beyond what would have been anticipated from current knowledge and solute transport models. It is hypothesized that these contaminants attach to small particles, called colloids, which may move relatively unhindered through the subsurface. Colloids with sizes between 1 nm and 1 µm can, under certain conditions, move large distances through a porous medium.

Considerable advances have been made in understanding colloidal processes and transport in well-defined systems such as water-saturated sand filters. However, key processes including colloid formation, mobilization, and deposition in different types of natural porous media are still not well understood. Although colloidal particles are naturally present in most soils, sediments, and rocks, they do not necessarily form stable suspensions and are therefore not very mobile. However, when certain system parameters are changed, such as the water flow rate or the solution chemistry, colloidal particles may become mobile and act as carriers for contaminants.

Microorganisms are a special class of colloidal particles. While their own fate and transport is strongly affected by their surface properties, microorganisms, like other colloids, can also alter the subsurface transport of organic and inorganic contaminants. For instance, microbial precipitation of soluble radionuclides and metals within cells or at cell surfaces can substantially alter the transport properties of these contaminants.

Knowledge of colloidal processes in the subsurface improves the accuracy and reliability of predictions of short- and long-term contaminant fate and transport. Also, natural augmentation or artificial introduction of colloidal particles, such as microorganisms, into the subsurface is a potentially promising new remediation technology for many types of contaminants. Long-term stewardship of waste sites and the development of appropriate remediation strategies require detailed mechanistic understanding of colloidal processes in the subsurface.

The specific mechanisms of colloid interactions with subsurface materials are not well understood. Nor is the transport of colloids in natural soils, sediments, and rocks. To describe quantitatively, and predict, the role and significance of colloids in contaminant transport, research must focus on three goals: (1) understanding mechanisms of colloid-contaminant and colloid-sediment interactions, including colloid formation, mobilization, and deposition; (2) improving sampling and analysis techniques for colloids and colloidal transport; and (3) modeling colloid transport and colloid-facilitated transport in unsaturated soils, sediments, and fractured rocks. The following three roadmap activities are directed at these goals. Table 4 highlights some major results that can be anticipated from these activities, given sufficient support and programmatic direction to accomplish the tasks listed under the activities.

Activity COL1. Improve sampling and analysis for colloids and colloidal transport.

- **Task with Near-Term Endpoint.** Develop a scientifically based protocol for field based sampling and analysis for colloids and colloidally transported contaminants.
- **Task with Near-Term Endpoint.** Develop new sampling techniques for *in situ* measurements of colloidal particles in pore water.
- **Near-Term Status Point.** Mobile colloids are considered in sampling and analyses protocols for field studies and monitoring systems.

Activity COL2. Studies of colloidal transport.

- **Task with Mid-Term Endpoint.** Quantify effect of preferential flow on colloid transport.
- **Task with Mid-Term Endpoint.** Understand relevance of colloid-facilitated transport to contaminant movement under transient flow conditions, including wetting, drying, and infiltration processes.
- **Task with Mid-Term Endpoint.** Quantify the potential for *in situ* colloid formation and mobilization under conditions relevant for major vadose zone contamination sites, particularly in the presence of extreme chemical conditions that can lead to dissolution and precipitation of soil minerals.
- **Task with Mid-Term Endpoint.** Evaluate the effects on production and behavior of microbial colloids of (1) changing contaminant flux, (2) nutrient injection during engineered bioremediation, and (3) cell to cell communication (quorum sensing) in biofilms and other cell assemblages.
- **Task with Mid-Term Endpoint.** Characterize colloid-contaminant interactions as a function of solution chemistry and water saturation, at both microscopic and macroscopic levels.
- **Task with Long-Term Endpoint.** Characterize colloid transport in different natural porous media relevant for sites with contaminated vadose zones. In particular, characterize and quantify colloidal transport through unsaturated fine and coarse sands and fractured rock, as a function of water saturation and

solution chemistry. Quantify colloid interactions with solid-liquid and liquid-gas interfaces.

Activity COL3. Models of colloidal transport.

- **Task with Long-Term Endpoint.** Model colloid transport and colloid-facilitated transport in unsaturated soils, sediments, and fractured rocks.
- **Long-Term Status Point.** Improved conceptual and mathematical characterizations of colloid-contaminant-soil interactions and colloid-facilitated transport have been incorporated into reactive transport models used by DOE and other agencies for assessing vadose zone contamination.

Table 4 Highlights of Results for Colloidal Formation & Transport Research Activities

	Near Term	Mid Term	Long Term
We know how to detect mobile colloids and how to sample and analyze them.	◆		
Important colloid-contaminant interactions understood at micro and macro levels.		◆	
Flow and transport models can map and predict important colloidal interactions and transport.			◆

2.6 Multiphase Flow and Transport

Multiphase flow and transport of organic and inorganic contaminants in the vadose zone poses serious scientific and technical challenges. The vadose zone always contains multiple fluid phases through which contaminants may move, as well as associated interfaces for partitioning between phases. For example when air, water, NAPLs, and an immobile solid phase are present, three mobile phases may occur, with as many as six interfaces for contaminant interphase mass transfer. The remediation of contaminated sites is ultimately controlled by the rates of these interphase mass transfers. Furthermore, migration and transport processes in the vadose zone control the rate of contaminant loading in the saturated zone.

Over the past several decades, research has focused on quantifying flow and transport processes using idealized fluids and porous media. This research has greatly improved overall knowledge and the ability to predict multiphase flow and transport. However, additional research is necessary to quantify the effects of subsurface physical and biogeochemical heterogeneity on contaminant fate and persistence. Procedures to scale laboratory-derived constitutive properties and parameters up to field scale are especially important. These include mass transfer and biological parameters that are typically measured at the soil column and microcosm scales. Unstable and preferential flow (e.g., fingering) of aqueous and NAPL phases is another important issue because of its potential to enhance contaminant mobility in the subsurface.

Additional difficulties arise when sites contain complex mixtures of inorganic and organic compounds, such as heavy metals or radionuclides mixed with organic solvents and complexing agents. Interactions among aqueous phase contaminants are known to influence their geochemical behavior and transport. Very little research has explored and quantified the fate and persistence in the vadose zone of contaminant mixtures that may involve complex interactions among phases, interfaces, and chemical components. These interactions will likely influence multiphase flow and transport processes, as well as bioavailability of contaminants. Related questions concern the effects of chelating agents and NAPL phases on heavy metal and radionuclide transport, differences in the transport of complex NAPL mixtures versus pure NAPLs, the effect of aqueous chemistry on NAPL migration and transport, and the potential adverse and synergistic interactions among contaminants in mixtures during remediation operations. Understanding the nature of the contaminant association increases the probability of developing efficient remediation strategies that treat multiple contaminants simultaneously.

As discussed in more detail in Sections 3.4 and 4.2, a combination of well-designed laboratory, numerical, and field-scale studies is required to test specific hypotheses related to multiphase fluids. Multidisciplinary teams are needed to address these complex issues effectively. Collaboration among disciplines would improve descriptions of multiphase flow and transport processes in complex vadose zone environments, thus reducing uncertainty and ultimately providing specific tools for the design and implementation of cost-effective remediation and containment operations.

The following three roadmap activities incorporate research needed to understand, measure, and model multiphase transport. Table 5 highlights major results that can be anticipated from these activities, given sufficient support and programmatic direction to accomplish the tasks listed under the activities.

Activity MP1. Extend knowledge and predictability of flow and transport processes to multiphase systems.

- **Task with Near-Term Endpoint.** Quantify effects of subsurface physical and biogeochemical heterogeneity on multiphase flow and transport processes.
- **Near-Term Status Point.** Upscaling procedures to apply laboratory-derived multiphase constitutive properties and parameters to the field scale have been developed.
- **Near-Term Status Point.** Process-based models can describe unstable and preferential flow of aqueous and NAPL phases.
- **Task with Mid-Term Endpoint.** Conduct multiphase flow and NAPL transport experiments for representative soils and contaminants, to elucidate real-world problems and data limitations.

Activity MP2. Studies of key contaminant mixtures (for DOE and other contaminated vadose zone sites) as multiphase systems.

- **Task with Mid-Term Endpoint.** Measure flow and transport properties of key contaminant mixtures. Refine theory and numerical models to describe their flow and transport in relevant subsurface environments.

- **Task with Mid-Term Endpoint.** Design, implement and analyze controlled tests of complex contaminant mixtures in highly heterogeneous systems.

Activity MP3. Incorporation of understanding and models for multiphase flow and transport into site assessments and remediation strategies.

- **Long-Term Status Point.** Remediation strategies routinely take into account multiphase flow and transport of site-specific contaminant mixtures.
- **Long-Term Status Point.** Numerical models are being used to assess uncertainty in flow and transport of complex contaminant mixtures at priority sites (including DOE sites) and to support decisions with regard to remediation and containment strategies.

Table 5 Highlights of Results for Multiphase Flow & Transport Research Activities

	Near Term	Mid Term	Long Term
We can model processes with unstable or preferential flow of aqueous and non-aqueous phases.	◆		
We can detect and interpret multiphase flow and transport of complex contaminant mixtures at contaminated sites.		◆	
Site assessment models incorporate multiphase flow and transport.			◆

2.7 Unstable Processes

Field observations of fluid flow and chemical transport in both porous and fractured unsaturated media often show unstable, spatially and temporally random fluctuations in the moisture content, pressure, flow rate, temperature, and concentration of chemicals. These fluctuations can result in rapid preferential flow and transport through the vadose zone to the groundwater table.

Despite numerous studies of preferential flow, many of the causes of flow instability are still not completely known. What is known, however, is that flow in structured, macroporous soils and fractured rocks is significantly influenced by abrupt changes in media physical properties (e.g., rough to smooth fractures, small to large pores) and by the interplay between gravitational and capillary forces. These interactions generate liquid fragmentation (bridges, fingers, rivulets), intermittent flow, and extreme sensitivity to small changes in boundary conditions and variations in media geometry. None of these phenomena are typical of homogenous porous media.

Other examples of processes leading to unstable and chaotic-type flow are discontinuities in the behavior of liquids in porous media. Examples include Haines jumps, flow-induced nonlinear effects in thin liquid films, drainage by cavitation, nucleation and mineral precipitation within pore spaces, density driven flow, dripping water in fractures and caves, fracture–matrix interaction processes, and thermal effects. Furthermore, combinations of several nonlinear physical processes involving both deterministic-chaotic and random flow and transport processes may cause spatial and temporal fluctuations of flow parameters. Continuum models have limited utility for representing inherently unstable and chaotic systems because of the need for different governing equations to describe intermittent flows in different parts of the system and at different times.

Chaotic dynamics is one of several new fields in modern science attempting to understand order and pattern in nature that cannot be explained with traditional linear deterministic theories. Recognizing the presence of deterministic chaotic processes may help to improve predictions of unstable flow and transport in the subsurface. In particular, chaotic dynamics may improve our understanding of the physics of unstable patterns of flow in variably saturated porous and fractured media, which can be described with either deterministic or stochastic models. For such a system, one can provide precise short-term predictions using deterministic-chaotic models; only a range of possible long-term predictions can be made using stochastic models.

To understand more thoroughly the physics of processes leading to unstable flow, special experimental and modeling investigations are needed. Models are needed to describe coupled, highly nonlinear processes of flow and mass transport in variably saturated media. It is also important to identify criteria (such as Bond and capillary numbers) that can be used to determine the onset of chaos.

Two roadmap activities incorporate research needed to understand and model unstable processes. Table 6 highlights major results that can be anticipated from these activities, given sufficient support and programmatic direction to accomplish the tasks listed under the activities. Other issues of nonlinear dynamics, involving coupled GHCB processes, are discussed in Section 3.1.2.

Activity UP1. Studies of factors influencing unstable flow.

- **Task with Near-Term Endpoint.** Identify directions for applying chaos theory in vadose zone hydrology by (1) reviewing the literature on physical, chemical, and biological processes in which unstable flow occurs; and (2) comparing processes and conditions in other environments with those occurring in the vadose zone.
- **Task with Near-Term Endpoint.** Perform bench-scale and field-scale investigations of factors leading to instability and chaotic-type flow and chemical transport in vadose zone conditions.
- **Near-Term Status Point.** Criteria have been developed to identify the onset of unstable and/or chaotic-type processes in vadose zone flow and transport.
- **Task with Mid-Term Endpoint.** To identify conditions for which unstable and/or chaotic-type processes are important, design and perform field-scale infiltration tests with tracers at several sites with vadose zone contamination in heterogeneous soils and fractured rocks.
- **Task with Mid-Term Endpoint.** To determine the main diagnostic parameters of chaotic-type flows, develop software that reconstructs the system phase-space from scalar data.

Activity UP2. Modeling unstable and chaotic flow in the vadose zone.

- **Task with Near-Term Endpoint.** Develop a series of models describing unstable flow phenomena of deterministic chaos in unsaturated fractured rocks.
- **Task with Mid-Term Endpoint.** Develop a new generation of mathematical and numerical models to describe unstable and chaotic-type flow processes in soils and fractured rocks.
- **Task with Long-Term Endpoint.** Implement models of unstable and/or chaotic-type flow into other deterministic and stochastic models used for predicting flow and transport and designing remediation activities.

Table 6 Highlights of Results for Unstable Processes Research Activities

	Near Term	Mid Term	Long Term
We can identify the onset of chaotic and unstable processes.	◆		
We can determine whether and when chaotic conditions are important at a site.		◆	
Site assessment models incorporate models for chaotic and unstable flow.			◆

3.0 COMBINING THE BASICS TO UNDERSTAND, MEASURE, MONITOR AND MODEL VADOSE ZONE SYSTEMS

As noted in Section 2.1, development of site-wide quantitative GHCB models, which can simulate the vadose zone of a contaminated site as an integrated system, is an arduous and iterative process. It requires concerted collaborations between numerical simulation of flow, transport, and transformational processes and the data collection necessary to initialize, constrain, and validate the models for these processes. What is necessary for more timely development is a toolkit for computations and interpolations that can scale data collected at different instrument support scales, data collected over varying time periods, and data collected at different spatial scales.

In this section, roadmap activities are discussed for important parts of that toolkit, beyond understanding, measuring, and modeling basic processes and properties within customary disciplinary boundaries. Section 3.1 examines research needed across disciplinary lines to characterize and model more realistically the coupled processes of vadose zone systems. Section 3.2 addresses research needed to measure and represent properties and processes at multiple spatial and temporal scales, a requirement for quantitative GHCB models. Section 3.3 describes work needed to estimate and reduce uncertainties in GHCB models. Section 3.4 deals with other issues in integrating and validating these models as site-wide representations of vadose zone systems.

3.1 Coupling Basic Properties and Processes

The separation of topics in Section 2 followed traditional disciplinary lines. This organization was arbitrary; it was used to simplify the presentation. In reality, variably saturated liquid flow, contaminant transport, and biogeochemical processes occur not in isolation but as tightly coupled systems often displaying nonlinear behavior. For example, fluid flow is the primary mode of transport for many contaminants in the vadose zone. However, the chemical makeup (concentration and ionic composition) of the fluid phase and various biogeochemical reactions can significantly affect fluid and solid phase properties, which in turn affect fluid velocities and rates of contaminant transport. Improved descriptions of the nonlinear transient interactions between the various processes and subsurface properties are needed, as are methods to deal with the overwhelming complexity of these processes. Integration is also essential for identifying which properties are the most relevant, and at what resolution, accuracy, and uncertainty they must be estimated for effective input to predictive models.

3.1.1 Coupling Process and System Models across Traditional Disciplinary Boundaries

Coupled models require an understanding of the complex interactions among mineral, microbial, and colloidal surfaces and among fluid, solid, and gas phases. Some of these processes include precipitation, surface complexation, sorption, attachment and detachment, multi-domain diffusion, oxidation and reduction (both inorganic and microbially mediated), porosity alteration, and heat flow occurring in a physically and chemically heterogeneous environment. Progress has been made in understanding individual processes at a basic level, but research prioritization is needed because of the many components and interactions involved. Fundamental understanding at a molecular level may allow a few components to be studied intensively and the results expanded to a wider class. In parallel, systematic study of coupled reaction systems in bulk phase media can improve understanding of these mechanisms and their manifestation on important coupled processes at the larger scales of observation.

It is important to realize that many problems in reactive transport modeling can be reasonably well addressed by understanding one dominant aspect of the problem. Nonetheless, models need to be available that incorporate all of the relevant processes, in order to select the appropriate interactions. Too often the model is selected first, and processes not included within that model are simply ignored.

Research needed for coupled models can be divided into database needs and constitutive theory needs, as well as computational resources and numerical algorithms. Roadmap activities for the first two are listed below. Computational resources, including numerical algorithms, are discussed in Section 4.3.

Activity CP1. Improve existing or develop new databases for processes with coupled GHCB properties

- **Task with Near-Term Endpoint.** Update and check reliability of available databases used in coupled models. Make the reliable databases universally available, with recommendations for usage.

Activity CP2. Develop cross-disciplinary modeling approaches and implement better models (representations) for key vadose zone flow and transport processes that cross traditional disciplinary boundaries.

- **Near-Term Status Point.** Better estimation techniques are available to facilitate routine incorporation into process models of different types of GHCB data that have different sampling scales and different spatial variability.
- **Near-Term Status Point.** Coupled processes with the highest priority for understanding vadose zone fate and transport, and the gaps in understanding them, have been identified.
- **Near-Term Status Point.** Model studies have demonstrated capabilities and limitations of existing coupled models. Procedures for their appropriate use have been codified and are widely disseminated and accepted. Strongly coupled nonlinear phenomena requiring development of new modeling approaches have been identified.
- **Task beginning in Near-Term, with Long-Term Endpoint.** Use the results from the identification of priority coupled processes and knowledge gaps

about them to guide research on sufficiently realistic representations of the highest priority processes.

The following status point applies to both activities in this section. Additional crosscutting status points for these activities are listed at the end of Section 3.1.2.

Long-Term Status Point (applies to Activities CP1 and CP2). Realistic representations of the priority coupled processes have been developed, validated in field studies, and implemented in vadose zone fate and transport models.

3.1.2 Understanding and Modeling the GHCB Aspects of Strongly Coupled Nonlinear Systems

For vadose zone modeling, strongly coupled systems are those where two or more fundamental geological, hydrologic, chemical, or biological processes must be understood and modeled together to accurately represent the flow and transport in the subsurface. Modeling of these coupled, often nonlinear systems is one of the most challenging problems in reactive transport. Examples include bioremediation; *in situ* redox manipulation for removal of chromium, uranium, and chlorinated hydrocarbons; coupled heat flow and transport for enhanced remediation or radioactively hot waste; and modeling the leakage of highly basic, highly radioactive tank waste solutions at Hanford or other DOE sites. Feedback between nonlinear processes can lead to instabilities. Examples include coupled chemical reaction fronts that can become stable or unstable, depending on the nature of the water chemistry and the mineralogy of the permeable material.

Conventional modeling techniques cannot handle truly coupled nonlinear processes. The current capability to model some of these processes is mostly limited to crude locally lumped parameter models that hide much of the complexity. More advanced models are available to model specific processes, such as adsorption, precipitation, or microbial transformation. Nonetheless, the basic scientific understanding of the processes, and especially of their couplings, is currently too weak for these models to be much more than useful tools for research. Developing a basic scientific understanding of the coupled processes themselves is a paramount goal when it comes to modeling this class of problems. Accurate and complete field and laboratory data are also needed to develop, test, and apply the improved models.

The roadmap activity below includes major tasks and significant status points for developing the understanding and modeling capability for strongly coupled nonlinear GHCB phenomena. Some of the status points refer to issues such as scaling and managing modeling uncertainty, which are discussed in later subsections of Section 3. Some status points refer to the vadose zone Problem Solving Environment (PSE), a software system environment and application toolkit discussed in Section 4.3.1.

Activity CP3. Develop realistic representations for strongly coupled nonlinear GHCB phenomena. Incorporate adequate models for these phenomena in transport models for vadose zone contamination sites.

- **Near-Term Status Point.** Models have been formulated for strongly coupled nonlinear GHCB phenomena with high priority for vadose zone contamination studies. The modeled phenomena may include mechanics of biofilms; multivariate reaction kinetics; saturation and colloid-facilitated transport; and scaling of coupled processes in space and time.
- **Mid-Term Status Point.** Constitutive theories and parameter databases for strongly coupled nonlinear GHCB systems have been improved and incorporated into vadose zone contaminant transport models.
- **Mid-Term Status Point.** Models for strongly coupled nonlinear systems have been linked with scaling techniques.
- **Mid-Term Status Point.** Mechanical-hydraulic and biochemical-hydraulic prototypes are available for use.
- **Mid-Term Status Point.** Models for strongly coupled nonlinear GHCB systems are supported in the PSE.
- **Task with Mid-Term Endpoint.** Test proposed models for strongly coupled nonlinear phenomena on synthetic test problems, in small-scale and meso-scale laboratory experiments, and at field-scale research sites.
- **Long-Term Status Point.** Improved computational algorithms are available for strongly coupled nonlinear GHCB processes.
- **Long-Term Status Point.** Models for strongly coupled nonlinear GHCB systems have been tested in field applications.

The following two status points apply to Activities CP1 through CP3.

Long-Term Status Point. Realistic models are available for all coupled GHCB phenomena, including strongly coupled nonlinear processes, that are important to vadose zone flow and transport. These models cover all important time and space scales, and most of them are available within the PSE.

Long-Term Status Point. Three-dimensional fully coupled heat and multiphase flow and transport models are the norm for decision support.

3.1.2.1 Highlights of Roadmap Results for Coupled GHCB Processes

Table 7 highlights some of the major results that can be anticipated from these three research activities for studying coupled processes. The time horizons indicated in the table are contingent on sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under the activities.

Table 7 Highlights of Results for Understanding and Modeling Coupled Systems Research Activities

	Near Term	Mid Term	Long Term
The highest priority coupled GHCB processes have been identified.	◆		
We understand the strengths and weaknesses of existing models.	◆		
Some of the important strongly coupled phenomena can be modeled.	◆		
Process models for important strongly coupled phenomena have been validated and field-tested across spatial and temporal scales.		◆	
Site assessment models incorporate all important coupled GHCB phenomena realistically.			◆

3.2 Combining Processes and Data at Different Scales in Integrated Models

Mathematical models of processes governing fate and transport in the vadose zone are constructed from mass, momentum, and energy balance statements. These statements depend on constitutive theories that define how flow and transport variables depend on material properties. Flow properties, including unsaturated hydraulic conductivity, water retention curves, and others, are defined for a specific spatial and temporal scale. A given process description, or the constitutive model representing it, does not explicitly incorporate processes at other spatial and temporal scales.

Conventional process descriptions/models such as the Richards equation for flow are established as useful representations for idealized uniform porous media. However, no such medium occurs in the natural subsurface. Many relevant subsurface properties exhibit multiple nested scales of variability in both space and time. As scale changes, the appropriate process description changes. The constitutive properties needed for modeling across scales are not uniquely defined. Consequently, constitutive theories relying on property measurements on one scale may be of little or no use to simulation on other scales affected by different flow and reactive transport processes.

Scaling issues affect boundary conditions, as well as the conceptual model and its parameters. Of special concern for vadose zone models is the temporal scaling of highly variable climatic forcing functions, especially given the wide range of time scales of interest for prediction, from a few years for remediation to millennia for stewardship. The critical questions in scaling include: (1) identifying the fundamental scales for different GHCB processes, (2) describing these processes at an observable scale, (3) identifying the relevant or pertinent spatial and temporal scales of concern for decision making, and (4) rescaling the processes to fit these parameters. The modeling exercise must also be concerned with how to capture the data needed to answer these questions.

Conventional scaling is often based on either physicochemical similitude over different scales or contrived assumptions about variability. Neither approach is adequate for fate and transport in structured soils and fractured rocks—media that are affected by discontinuities and preferential flow phenomena. Research on scaling must address not only the multi-scale nature of GHCB processes and the basic properties that control them. It must also accommodate the disparate scales of observations for characterization and for monitoring fate and transport. (Monitoring scales may be determined by regulations unrelated to the scale of the controlling phenomena.)

The major endpoints envisioned for general improvements in modeling capability are multidisciplinary scaling of constitutive theories; massive enhancements in deterministic and stochastic scaling tools; hierarchical frameworks for multiple scales of observation/measurement; and comprehensive error analysis and adaptive scaling methods. Among the focus areas for research are non-isothermal fate and transport, the occurrence and impact of preferential multiphase flow in the vadose zone, fate and transport in fractured media, and scaling episodically transient reactive transport in multi-scale heterogeneous media via generalized coordinate systems. Both general and focused research efforts must incorporate experimentation and measurements on appropriate scales to test and validate scaling strategies in realistic environments. Finally, the scaling results must be linked to the PSE and to advances in numerical methods (see Section 4.3).

Activity SC1. Develop simulation tools for vadose zone systems that provide a hierarchy of constitutive theories and that can simultaneously accommodate multiple processes on different scales.

- **Near-Term Status Point.** A Monte Carlo prototype for massive deterministic simulations of scaling issues has been designed and developed.
- **Task Beginning Near-Term with Mid-Term Endpoint.** Develop extensions of the massively deterministic Monte Carlo method to include probabilistic specifications of properties and constitutive hypotheses.
- **Mid-Term Status Point.** The extended Monte Carlo modeling capability is in use as a testbed for evaluating scaling approaches and for advanced quantification of errors associated with information loss in scaling.
- **Near-Term Status Point.** Scaling is being used to provide quantification of relevant processes by identification of global system variants, such as contaminant trajectories and travel times, non-aqueous mobile phase geometries, cumulative reaction histories over multiple time scales, and subsurface ecosystem dynamics.
- **Near-Term Status Point.** New deterministic and probabilistic/stochastic approaches have been developed to address cross-scale issues that commonly arise in vadose zone reactive flow and transport.
- **Task Beginning Near-Term with Long-Term Endpoint.** Undertake research to understand the time scaling of reaction systems and to solve problems of transients, episodic behavior, and boundary conditions.

- **Task with Mid-Term Endpoint.** Refine computational techniques for solving hierarchically scaled flow and transport models; test these techniques with meso-scale laboratory experiments, small scale field experiments, or other types of measurements of coupled GHCB processes.
- **Task with Mid-Term Endpoint.** Develop scaling methods for flow in generalized (transient and spatially non-uniform) coordinate systems to accommodate processes that vary on multiple spatial and temporal scales.
- **Mid-Term Status Point.** Research has provided linkages from constitutive theories and scale of measurement to the quantities of ultimate concern to decision-makers. These linkages are in use for planning and implementing characterization and monitoring activities.
- **Mid-Term Status Point** (also a status point for Activity PSE2, in Section 4.3.1). Models for strongly coupled nonlinear GHCB systems are supported in the PSE.
- **Task Beginning Mid-Term with Long-Term Endpoint.** Develop links between the scaling methods described above and the methods for uncertainty estimation and reduction in the PSE.
- **Long-Term Status Point.** Research is being done on spatial and temporal scaling in support of source-identification, as well as other inverse problems.
- **Long-Term Status Point** (also applies to Activities CP1 through CP3 for coupled GHCB phenomena). Strongly transient coupled GHCB processes at applied field sites can be modeled over multiple time horizons.
- **Long-Term Status Point.** Aspects of scaling theory have been unified and completely linked with methods for uncertainty estimation and reduction in the PSE.

Table 8 highlights major results that can be anticipated from this research activity, given sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under it.

Table 8 Highlights of Results for Combining Processes & Data at Different Scales Research Activities

	Near Term	Mid Term	Long Term
We can simulate scaling problems of important GHCB phenomena using probabilistic modeling.	◆ (end)		
We can measure and model coupled GHCB phenomena across spatial scales.		◆ (end)	
Site models incorporate strongly transient and coupled GHCB phenomena for multiple time periods.			◆ (end)
Site models incorporate scaling with estimates of uncertainty, and the models can propagate uncertainty estimates across spatial and temporal scales.			◆ (end)

3.3 Estimation and Reduction of Uncertainty

Uncertainty will always remain an issue with vadose zone models of flow and transport, if for no other reason than the vadose zone is heterogeneous and difficult to characterize and monitor. Uncertainty comes from the incomplete answers to two fundamental questions with which models must deal. First, what is an appropriate conceptual model for the intended purpose, one that is neither too complex nor too simplistic? Second, what are appropriate model parameters (e.g., properties), initial conditions, and boundary conditions? The answers to these questions depend, respectively, on fundamental research on processes and process coupling and on characterization and monitoring techniques. In addition, it is possible that subsurface systems also have an intrinsic or irreducible uncertainty, due to the spatially and temporally stochastic aspects of GHCB processes and the difficulty of observing these processes without completely dissecting the system. How then is uncertainty traced through the model and converted into quantities that decision-makers can understand, trust, and use?

Uncertainty in initial conditions, boundary conditions, and other model parameters is now treated primitively, if at all. Spatial variability of some flow parameters is sometimes simulated by generating simplistic alternative geologic realizations using stochastic methods or by running Monte Carlo realizations. Recently, these realizations have been conditioned by invasive and non-invasive monitoring and characterization data, which is an improvement. Temporal variability due to climate changes can be treated similarly, although historical records are often used instead of current data. More commonly the flow is considered to be steady (independent of climatic fluctuation).

Most uncertainty stemming from the choice of a conceptual model is dealt with informally, by an ad hoc process of deciding whether or not the model is “good enough.” While formal inverse approaches to estimate parameters are being developed, there has been much less attention paid to estimating boundary conditions (e.g., climate, meteorology, contamination source), and almost none to estimating appropriate conceptual models. Some conceptual models are useful for answering certain questions but fail miserably in attempting to answer others. An appropriate conceptual model depends not only on the system but also on the questions being asked—it must be pertinent.

Although Monte Carlo simulation is a computationally expensive method, it demonstrates that uncertainty estimation is possible. Further, the use of conditioned Monte Carlo realizations demonstrates that adding data can reduce uncertainty. Monte Carlo simulation will always be an appropriate tool for some vadose zone applications, but more computationally (and theoretically) efficient alternative analyses for sensitivity or uncertainty are needed, possibly based on more sophisticated probabilistic approaches.

Heterogeneity is a major source of uncertainty in vadose zone models. New theories for describing and understanding the spatial and temporal structures of naturally occurring heterogeneities and fluctuations are needed. Existing theories have not yet contributed much to solving basic science or engineering problems. New links are needed between probabilistic description of the media and probabilistic measures of flow and transport.

Improving the capacity to estimate and reduce uncertainties will lead to substantial increases in confidence in our ability to make good decisions regarding remediation, waste handling, or long-term stewardship. Models and approaches are also needed that can automatically alert the user to possible limitations caused by uncertainty, just as can be done for numerical error. For example, a modeling system could recognize that the conceptualization and the data are inconsistent (well beyond reasonable limits), suggest possible explanations for the inconsistency, and even adapt corrections itself. With formal uncertainty analysis and reduction methods, it should be possible to predict the value of new data, optimize the design and operation of characterization and monitoring activities, and update a model automatically when new data become available. These developments in uncertainty estimation, reduction, and application should be incorporated into the PSE (see Section 4.3.1).

Activity UC1. Catalogue, assess, and prioritize R&D needs for addressing the different sources of uncertainty in models of vadose zone flow and transport.

- **Near-Term Status Point.** State-of-the-art methods of uncertainty estimation and reduction, especially for risk analyses, have been catalogued and assessed.
- **Near-Term Status Point.** Sources of uncertainty in vadose zone modeling, including choice of conceptual model, geological heterogeneity; parameter values; and initial and dynamic boundary conditions, have been quantified and R&D needs to address them have been prioritized
    - Uncertainties contributed by geological heterogeneity in porous media have been quantified and R&D needs prioritized.
    - Uncertainties contributed by dynamic boundary conditions related to weather and climate variability and predictability have been quantified and R&D needs prioritized.
    - Uncertainties contributed by characterization and monitoring methods, including sample size, sample frequency, etc., have been quantified and R&D needs prioritized.
    - Uncertainties contributed by conceptual models of processes, especially overly simplistic or incorrectly scaled process models, and incorrectly coupled processes have been quantified and R&D needs prioritized.
- **Task with Mid-Term Endpoint.** Develop and test new theories and methodological approaches for describing and understanding the spatial and temporal structures of naturally occurring heterogeneities and fluctuations. Use advanced geological modeling to capture both flow-sensitive and chemical spatial heterogeneity.
- **Mid-Term Status Point.** Uncertainties for flow models of highly heterogeneous porous and fractured media, affected by the fracture-matrix

interactions and by film flow in dry formations, have been identified and evaluated.

Activity UC2. Research to decrease uncertainties in vadose zone modeling.

- **Task with Near-Term Endpoint.** Analyze existing long-term geological, hydrologic, chemical, and biological records to improve conceptual models, reduce their uncertainties, and reduce or quantify the uncertainties in estimates of parameters and boundary conditions used in vadose zone models.
- **Task Beginning Near-Term with Mid-Term Endpoint.** Test candidate methods for uncertainty estimation and reduction, and applications of these methods, on synthetic test problems, small-scale and meso-scale laboratory experiments, and field-scale research sites.
- **Task with Mid-Term Endpoint.** Evaluate effects of uncertainties for invasive and noninvasive field characterization and monitoring methods with different scales and degrees of resolution.
- **Mid-Term Status Point.** Uncertainty estimation and reduction methods resulting from the Activity UC2 tasks with mid-term endpoints (see above) are in use as standard practice at several typical sites with vadose zone contamination.
- **Mid-Term Status Point.** New, more sophisticated and efficient probabilistic approaches to uncertainty estimation and reduction have been developed and tested.
- **Mid-Term Status Point.** Uncertainty estimation and reduction methods are in use to predict the value of new data, to optimize the design and operation of characterization and monitoring activities, and to automatically update a model when new data becomes available.
- **Task with Long-Term Endpoint.** Develop uncertainty and inverse methods that self-adaptively suggest modified conceptualizations or parameterizations.
- **Long-Term Status Point.** Forward and inverse models accounting for uncertainty are fully integrated into the vadose zone PSE.

Activity UC3. Improve computational methods for representing and propagating uncertainties in vadose zone models.

- **Near-Term Status Point.** Numerical algorithms have been improved to increase the efficiency of vadose zone Monte Carlo simulations.
- **Mid-Term Status Point.** More realistic treatment of uncertainties caused by surface boundary conditions have been incorporated in vadose zone models.
- **Mid-Term Status Point.** Support for uncertainty analyses has been incorporated in the vadose zone PSE.
- **Mid-Term Status Point.** Methods to display the degree of uncertainty from different sources and in aggregate (processes, coupling, parameters and

properties, variability, etc.) have been developed and incorporated in vadose zone system models. These methods exploit advanced visualization techniques and other sensory (e.g., sound and touch) interactions with models and data.

- **Mid-Term Status Point.** Users of vadose zone system models are automatically alerted to possible limitations caused by uncertainty.
- **Task with Mid-Term Endpoint.** Link the analysis of modeling uncertainty with practical problems of a facility designer. Integrate uncertainty estimation and reduction with estimation and reduction of numerical errors. Incorporate these modeling improvements into the vadose zone PSE.
- **Mid-Term Status Point.** Uncertainty analysis has been coupled to management models and the vadose zone PSE to help make decisions concerning characterization, monitoring, and remediation design and operation.

The following two long-term status points apply to all three activities for uncertainty estimation and reduction. The first also applies to roadmap activities for modeling coupled GHCB processes (see Section 3.1).

Long-Term Status Point (applies to Activities UC1–UC3 and CP1). Uncertainty estimation techniques are incorporated in commonly used biogeochemical models and models of multiphase flow in fractures.

Long-Term Status Point (applies to Activities UC1–UC3). Uncertainty estimation and reduction are standard practice and are in use for characterization, monitoring, remediation, and stewardship decisions.

Table 9 highlights some of the major results that can be anticipated from these three research activities for measuring and reducing uncertainty. The time horizons indicated in the table are contingent on sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under the activities.

Table 9 Highlights of Results for Estimation & Reduction of Uncertainty Research Activities

	Near Term	Mid Term	Long Term
We have identified and understand the sources of uncertainty for monitoring and modeling vadose zone sites.	◆		
We have assessed and catalogued the state-of-the-art methods for estimating and reducing uncertainty.	◆		
We have developed and tested new probabilistic approaches for estimating and reducing uncertainty.		◆	
We can optimize characterization and monitoring systems to reduce uncertainty, and we can predict the value of additional data for reducing uncertainty.		◆	
Site assessment models incorporate techniques for estimating and reducing uncertainty in making decisions on site cleanup and stewardship.			◆

3.4 Improving Site Monitoring Systems

To this point in the roadmap, *characterization* and *monitoring* have been generally paired, since both share many of the same tools and methodologies used to determine vadose zone processes and measure vadose zone properties. An effective monitoring program and a site-wide assessment performed with an integrated system model for a contaminated site complement each other and are equally important. In this section, the two are separated, in order to focus on the technology needed to improve site-monitoring systems.

The Executive Committee believes that monitoring capabilities for vadose zone sites must be a significant focus of roadmap activities. The committee foresees the thorough testing and adoption of improved methods for monitoring contaminated sites as one of the two overarching, high-value payoffs from implementing the research and infra-structure-building activities in the roadmap. In fact, monitoring systems will benefit from many of the near-term and mid-term results of the roadmap activities, and thus provide an important payoff even sooner than integrated system modeling may. New monitoring tools and methodologies will be integral parts of site restoration and remediation in the near term, as well as on longer time horizons. These new tools and methodologies will provide a backbone for long term stewardship, in which monitoring will be an essential element in verifying that vadose zone contaminants have been removed or stabilized and that migration toward groundwater aquifers is not occurring.

This section begins by distinguishing monitoring from characterization. Then it describes the fundamental goals of monitoring and the basic requirements for a monitoring system. From this background, the section ends by specifying the technology needed for developing new monitoring methods and the roadmap activities to produce that technology.

3.4.1 Monitoring Distinguished from Characterization

Characterization is typically associated with the initial investigation of a site. Characterization data are often collected to identify how much of which contaminants are located where, as well as to provide a three-dimensional visualization of the structural geology and hydrogeology of the site. Equally important is the characterization of boundary conditions, such as precipitation and temperature, and how these conditions change with time. This initial visualization of the site often interprets the measurements collected by reference to conceptual models of the subsurface strata and the GHCB processes likely to be present. Quantitative models of individual or combined processes and conditions may be initialized or parameterized with the characterization data, to aid in the visualization effort.

Monitoring typically begins after a site has been characterized, to detect changes in the location and concentrations of contaminants or changes in other GHCB conditions that could affect contaminant fate and transport. Site monitoring is usually closely linked with environmental cleanup and/or stewardship activities at the site, and the monitoring program typically must be reviewed and approved by an environmental regulator and other stakeholders. As with the initial visualization during site characterization, monitoring requires a systematic approach that incorporates measurement tools with optimization approaches, scaling and uncertainty analyses, and modeling of contaminant fate and transport.

3.4.2 Progressive Steps for a Monitoring System at a Contaminated Vadose Zone Site

Monitoring is a significant and essential component of any approach to site environmental cleanup or stewardship. Table 10 lists the progressive steps for establishing, operating, and completing a monitoring program. These steps address four basic questions: **Where, What, How** and **What-if?**

- **Where?** The locations at which measurements are to be made, including locations to track the presence of contaminants and locations that are required to be within a standard of compliance.
- **What?** The vadose zone processes, contaminant species, and possibly surrogates (tracers or other indicators of contaminant transport) for which measurements are made to verify that the objectives of the approved site cleanup/stewardship plan are being met or to trigger a contingency plan.
- **How?** The techniques to be used for monitoring, the time scales, and the frequency of measurements in the monitoring program.
- **What-if?** The action levels, reporting requirements, and contingency plans if the approved cleanup/stewardship activities for the site fail to keep contaminants within standards at the points of compliance.

Table 10 Progressive Steps for a Monitoring System and Program to Accompany Federal Facility Cleanup and/or Stewardship Activities

Step	Description	Parties Involved
1. Establish **where** monitoring will be located	Specify points of compliance and other points at which monitoring measurements are made.	Regional Administrator
2. Define **what** is to be monitored	Demonstrate that approved cleanup/stewardship activities (e.g., contaminant removal, natural attenuation, barrier cover) are achieving expected results by including steps to: 1. Identify any potentially hazardous contaminants, including transformation products; 2. Determine if a plume is expanding (either down-gradient, laterally or vertically); 3. Ensure no impact to down-gradient receptors; detect new releases of contaminants to the environment that could impact the effectiveness of the planned remediation ; 4. Demonstrate the efficacy of institutional controls to protect potential receptors; 5. Detect changes in environmental conditions (e.g., hydrogeologic, geochemical, or microbiological) that may reduce the efficacy of any of the processes required for cleanup/stewardship to succeed; and	Site Operator and Regional Administrator

Step	Description	Parties Involved
	6. Verify that cleanup/stewardship objectives are being achieved.	
3. Establish the time period for monitoring (part of **how**)	Monitoring period should continue as long as contamination remains above required cleanup levels and continue for a specified period (e.g., 1–3 years) after cleanup levels have been achieved to ensure that contaminant levels are stable and remain below target levels.	Regional Administrator
4. Define how monitoring is to be done	Demonstrate monitoring approach is appropriate and can be accomplished verifiably by including steps to: 1. Specify methods for statistical analysis of data, e.g., established tolerances, seasonal and spatial variability; 2. Establish performance standards, such as: • Collection and evaluation of performance monitoring data for remediation methods in use at the site; • Monitoring natural attenuation performance; • Standard test methods. Currently available standard methods include those from the American Society for Testing and Materials (ASTM) and EPA standard methods.[a] 3. Establish a time interval agreed upon by regional administrator or agency. Include reporting maps, tabulation of data and statistical analysis, identification of trends, recommendations for changes in approach, evaluation of whether contaminants have behaved as predicted or other remedies are required.	Site Operator and Regional Administrator
5. Define action levels or processes to be observed for monitoring (part of **how**)	Establish metrics for the monitoring system by including steps to: 1. Establish background levels; 2. Define what criteria shows that a plume is expanding or diminishing; 3. Define what criteria shows that the conceptual model is applicable to a site; and 4. State the metrics of cleanup objectives and effectiveness.	Site Operator and Regional Administrator
6. Define actions to be accomplished when action levels or processes are observed (**what if**)	Establish action plan by including steps to: 1. Observe requirement to report to responsible party or agency if statistically significant variance occurs, compared to background; 2. Identify extent and nature of non-predicted behavior (e.g., release); 3. Reevaluate conceptual model; and 4. Evaluate feasible corrective actions from previous and evolving contingency plan.	Site Operator will provide details of the monitoring program to EPA or the State implementing agency as part of any proposed monitored natural attenuation remedy.

[a] Applicable ASTM standards include Soil Pore-Liquid Monitoring (D 4696-92); Time Domain Reflectrometry (D 6565); and Horizontal Applications of Neutron Moderation (D 6031). For further listings and details, see Table 3.3, page 169, in Looney and Falta, 2000, or the ASTM website, <www.astm.org>. Representative EPA documents include EPA 1994a, 1994b, 1997, and 1999 in the Reference section of this report.

Accomplishing the steps needed to establish improved monitoring system will depend on the confluence of many diverse technology paths in this roadmap. For example, new monitoring approaches will require constant and rapid upgrading of sensors, field optimization, and modeling methods.

The monitoring locations for a federal facility are chosen by the Regional Administrator (EPA or the State implementing agency), preferably using site characterization data and the conceptual model (understanding) for contaminant fate and transport at the site. These locations typically include *the points of compliance,* which are the locations at which observation of a process or attainment of a standard can verify the action of the remediation approach. Monitoring locations are also selected to allow contingency actions to protect human and environmental safety if an action level is exceeded (the **what if** question).

In the future, the importance of allowing a "monitoring margin" for contingency actions to protect groundwater resources is likely to move monitoring systems and plans toward selecting points of compliance located between the contaminant source and the groundwater. This imperative to protect the groundwater resource will place more emphasis on vadose zone monitoring. As noted in the Introduction, the alternative of controlling the groundwater within a contaminated zone is proving to be both more expensive and less effective than containing contaminants within the vadose zone.

The **how** question includes demonstrating that the monitoring approach is appropriate and verifiable.

3.4.3 Foundations for New Monitoring Approaches: Portfolio of Conceptual Models, Monitoring and Characterization Data

Long-term monitoring of vadose zone contamination must verify contaminant isolation by reliably detecting unintended releases. Monitoring must also detect changes in geological, hydrologic, chemical, and biological parameters and process rates. These capabilities should be developed through an iterative process, continually updating site conceptual models with new monitoring data and interpretation. New and continuing monitoring data will be invaluable in defining and confirming conceptual models; the data will also aid in determining the continued value of a particular model.

It is essential to link monitoring explicitly to contaminant fate and transport models before monitoring starts, so that subsequent monitoring efforts achieve their purpose. To facilitate this linkage, a portfolio of models, grouped by contaminant type, should be developed. Grouping by contaminant type has proven to be a good way of organizing this approach. Such portfolios and system knowledge gathered from them provide the foundation to answer the basic questions of **what, where, how**, and **what-if**.

There should also be an effort to cull from the set of standard monitoring approaches those that cannot conceivably update or refine the catalogue of chemical fate and transport models of a specific contaminant. This culling is important for minimizing data collection that is likely to be of decreasing value (orphaned data) as iterative improvement of monitoring systems and site models progresses.

Activity MON1. Build, catalogue, and update conceptual models for fate and transport of vadose zone contaminants, using field data on specific contaminant plumes to select and improve models for the catalogue.

- **Near-Term Status Point.** At least 2 or 3 conceptual models for fate and transport of particular contaminants, including contaminants of particular interest to DOE, have been built, catalogued, and updated using field data on specific contaminant plumes from DOE sites or other vadose zone contamination sites.
- **Mid-Term Status Point.** Field measurements from within and outside the DOE complex have been compiled to provide broad-based technical support for the catalogue of fate and transport models. Characteristic transport distances, chemical controls on attenuation, and hydrologic factors have been determined on a site-specific basis, but these features have been used collectively to update the conceptual models in the catalogue.
- **Mid-Term Status Point** (also applies to Activity MON3). Contaminant-specific monitoring needs have been catalogued. Current "standard" monitoring approaches that cannot conceivably update or refine the catalogue of conceptual models for attenuation of a specific contaminant have been identified.

Activity MON2. Coordinate effort to collect long-term monitoring lessons learned from across DOE sites and from other agencies with monitoring experience and expertise.

- **Task with Long-Term Endpoint.** Use the gathered monitoring data and lessons learned to institutionalize a reflexive and iterative linkage between monitoring and model refinement
- **Task beginning Mid-Term with Long-Term Endpoint.** Use the gathered monitoring data and lessons learned to (1) condense the catalogue of conceptual models for contaminant attenuation/fate and (2) standardize monitoring approaches.

3.4.4 Contaminant Fate and Transport Monitoring

Many of the remediation alternatives for existing contaminated sites or decommissioned facilities will leave residual wastes in place. Such residual or stabilized contaminants require assessment of their potential to migrate through the vadose zone. Methods for monitoring these potential sources are important because, once wastes are released to the heterogeneous subsurface, containment is extremely problematic and remediation is very expensive. A huge gap exists between the state of the art in implementing monitoring systems and the state of practice at most sites of significant vadose zone contamination, including the DOE cleanup sites. This gap needs to be narrowed. Also, new monitoring approaches are an integral part of verifying the effectiveness of remediation, including triggering and defining appropriate contingency actions (addressing the **what-if** question).

To date, there have been limited studies of non-invasive and non-point methods of identifying and monitoring contaminants. There are currently no techniques for monitoring real-time changes in source contaminant configuration (e.g., migration of contaminants in the vadose zone below disposal cribs or tanks).

Activity MON3. Define monitoring requirements and improve/develop monitoring approaches for chemical contaminants, including changes GHCB frameworks and boundary conditions.

- **Near-Term Status Point.** Integrated field-tests of integrated (multiple sensors, system optimization, coupled to conceptual models) monitoring systems at integrated field-test sites or actual site undergoing remediation or in closure stage. Begin incorporation of new sensors into monitoring system
- **Mid-Term Status Point.** A cost-effective real-time monitoring and data analysis system has been developed that provides early warning of contaminant discharges to the vadose zone.
- **Mid-Term Status Point.** New sensors and emplacement methods can be incorporated cost-effectively into monitoring systems, to move state-of-the-art technology into the state of practice at cleanup and stewardship sites.
- **Mid-Term Status Point.** Contaminant-specific monitoring needs have been catalogued. (See related status point for Activity MON1.)

3.4.5 Highlights of Roadmap Results for Improving Site Monitoring Systems

Table 11 highlights some of the major results that can be anticipated from the three research activities for improving site monitoring systems. The time horizons indicated in the table are contingent on sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under the activities.

Table 11 Highlights of Results for Improving Site Monitoring Systems Research Activities

	Near Term	Mid Term	Long Term
Several conceptual models for fate and transport (beginning a catalogue) have been validated with field data representing an emerging set of standard monitoring approaches.	◆		
Researchers, site operators, regulators and stakeholders can access a catalogue of proven fate and transport models with data sets for priority vadose zone cleanup sites.	◆		
Real-time monitoring systems at sites with vadose zone contamination provide early warning of contaminant discharge or movement.		◆	
The model catalogue has been condensed and updated, and monitoring approaches have been standardized.			◆

3.5 Model Integration and Validation at the System Level.

To address the national problems of vadose zone contamination, the processes and properties that control flow, transport, and transformations must be understood, measured, and ultimately incorporated in validated predictive tools whose results affect remediation and stewardship decisions. Data from myriad characterization techniques, both non-invasive and invasive, will likely be integrated over many iterative cycles to achieve site-specific multidisciplinary models whose predictions (summary results of simulation runs) consistently honor all data and their uncertainties.

Rigorous testing of model output, or predictions, is critical to building confidence in the characterization methods and data, as well as validating the conceptual models and numerics incorporated in the integrated models that produce the predictions. Quantities simulated by mathematical models (e.g., pressure and concentrations) are more readily measured than are many model input parameters (e.g., boundary conditions like infiltration, or properties like hydraulic conductivity and porosity). These simulated quantities are therefore often easier to test in controlled experiments or in the field.

By contrast, estimates of model input parameters are often made using inverse modeling, an approach plagued by problems of instabilities, non-sensitivities, and non-uniqueness. In addition, parameter estimation procedures are still frequently used without probabilistic representations to account for the uncertainties in these procedures. The resulting "point value" parameter estimates are rather meaningless, since not much can be said about the relationship between the estimated and true parameter values. Consequently, the underlying uncertainty in the estimates cannot be propagated in a reasoned way into estimates of the uncertainty, or the sensitivity, of predictions from the integrated model. Data collection programs are still regularly designed without studying beforehand the sensitivities of key model input parameters to measured variables.

These limitations constrain the capacity to test and validate a model thoroughly. The constraints are particularly serious when the model is to be used for long-term predictions. For such uses, even though model output may be measurable in principle, it cannot be tested, and therefore validated, until years after critical decisions have been made and acted upon. To address these limitations, requirements for integration and validation must be designed into each step of the process and rigorously implemented.

The modeling process consists of the following four general steps: (1) develop a conceptual model, (2) formulate a mathematical model, (3) implement solution techniques, and (4) perform model verification and testing. Errors in the conceptual model can lead to errors in predicting and understanding vadose zone flow and transport. Alternative conceptual models are proposed when lack of data or process understanding precludes unique identification of a single model, site characterization defines a new feature or process, or model testing rejects a candidate conceptual model. A major barrier to identifying alternative conceptual models is the design and execution of experiments that discriminate among various models.

Definition models must be integrated with data from characterization and monitoring activities. The resulting site-specific description of a vadose zone system must be validated to ensure that a model is performing adequately for its intended uses. The data needed to test the models can come from a variety of sources.

- Synthetic (computer-based) test problems provide the only data sets in which all aspects of the system are known.

- Integrated meso-scale laboratory and field experiments provide a higher level of realism, but with gaps in even the most exhaustive database.
- Finally, applying the model to site studies provides the ultimate reality test, but leaves even larger data gaps.

Integrated system models should be tested and validated in each of these test environments. Special attention should be paid during testing to comparative studies of various approaches to inverse modeling and estimation.

To improve integrated system models and assist with integration, new inversion techniques must be developed to estimate parameters and boundary conditions. Traditionally parameters (e.g., properties) have received the most attention, usually under steady-flow assumptions. Transient data generally reduce the uncertainty in parameter estimates and can overcome problems of identification. The new methods should couple transient flow and transport processes, together with other characterization information, in large-scale joint inversions. As part of the PSE (see Section 4.3.1), it would be useful to establish a computational test bed to validate models consistently against relevant data.

Using the synthetic problems, well-controlled meso-scale experiments, site data, and possibly other means, integrated system models should be tested and validated with respect to three major criteria:

1. Does the model consistently honor all available data and understanding of processes?
2. Are the model and data adequate to make the desired predictions?
3. Where would new or additional data most likely improve model performance?

New measures of model performance, based on these criteria, are needed.

To apply integrated system models to sites, the entire modeling approach should be integrated with data through an appropriate geographical information system (GIS). The GIS should provide tools and methods for managing data in space and time, including special interrelationships and uncertainties. Such GIS tools could be an integral part of the PSE or simply linked to it. Site considerations also suggest the design, building, testing, and updating of a shared vadose zone model that contains a subset of features of the PSE sufficient for dealing with most vadose zone problems. It, rather than the parent PSE, could become the main vehicle for model application and decision support at sites.

The following four roadmap activities address these needs for integration and validation throughout the stages of designing, implementing, and applying a site-wide integrated system model for priority vadose zone sites, such as the long-term DOE cleanup and stewardship sites. Table 12 highlights major results that can be anticipated from these activities, given sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under them.

Activity IV1. Improve and test techniques: (1) for estimating model input parameters, including boundary conditions and properties that control flow and transport and, (2) for model integration, through improved measurement system design and/or improved inverse modeling of input parameters.

- **Task with Near-Term Endpoint.** Develop models of sampling events and instrument response, to be used to improve instrument design, for a variety of invasive and non-invasive methods for characterization and monitoring.
- **Task with Near-Term Endpoint.** Develop new inversion techniques for estimating the input parameters in models of transient flow and transport processes.
- **Task with Long-Term Endpoint.** Design and conduct controlled field experiments that distinguish among conceptual models representing different sides of issues in vadose zone flow and transport.
- **Mid-Term Status Point.** Improved methods for inverse modeling and estimating probabilistic uncertainty have been tested through meso-scale laboratory and field-scale experiments.
- **Long-Term Status Point.** A highly integrated Shared Vadose Model has been developed, validated, and is being applied. This model is a subset of the PSE in which the value of new data is continually assessed as part of an observation–prediction–decision support (cost analysis) process.

Activity IV2. Develop new tools to test and validate vadose zone models and techniques, such as inversion methods, for integrating data and estimating key parameters.

- **Task with Near-Term Endpoint.** Define synthetic test problems and use them to conduct comparative studies of existing techniques for inverse modeling and model validation.
- **Mid-Term Status Point.** Integrated meso-scale laboratory and field experiments have been performed to build databases suitable for testing and validating specific models.
- **Mid-Term Status Point.** A computational test bed to assist in testing and validating models has been incorporated into the vadose zone PSE.
- **Mid-Term Status Point.** Support for inverse methods and for decision support simulations has been added to the PSE.
- **Mid-Term Status Point.** Geographical information systems have been linked with, or otherwise functionally incorporated into, the PSE.

Activity IV3. Conduct vadose zone field experiments to test and refine models and measurement techniques, including advances in instrumentation, tracers, biological properties, and emplacement technologies, as well as mathematical and statistical bases for design.

- **Long-Term Status Point.** Models can be tested by comparing model predictions to short-term (and eventually long term) field observations from field test sites and monitoring networks at contamination sites.

Activity IV4. Apply improved methods and tools for integration and validation to real-world problems of managing vadose zone contamination.

- **Mid-Term Status Point.** Model testing and validation methods are being applied at major vadose zone contamination problems, including DOE sites.
- **Long-Term Status Point.** Better inverse methods for estimating parameters, boundary conditions, and the uncertainties in these estimates, and better methods for conceptual model validation, have been developed and validated using synthetic problems, experiments, and site data. They are being used to guide characterization and monitoring activities at sites with major vadose zone contamination problems, including DOE sites.

The following status point applies to all four Integration and Validation activities.

Long-Term Status Point (applies to Activities IV1–IV4). Models are an effective bridge to visualize and communicate findings from scientists to policy-makers and stakeholders.

Table 12 Highlights of Results for Integrating and Validating Site-Wide Models Research Activities

	Near Term	Mid Term	Long Term
We can compare modeling techniques using a standard set of synthetic test problems.	◆		
We have models for sampling events and instrument response to improve instrumentation and network design for characterization and modeling.	◆		
We can test and validate models and measurement methods in laboratory and field experiments following standard protocols.		◆	
Site-wide assessment models are credible to both scientific and public policy communities.			◆

4.0 NECESSARY SUPPORTING CAPABILITIES AND INFRASTRUCTURE

The results of the research activities outlined in Sections 2 and 3 will be improvements in our understanding and our capability to monitor and model the fate and transport of subsurface contaminants. To pursue these activities effectively and achieve the anticipated results within the time horizons indicated, researchers and developers need capabilities and facilities that do not yet exist. Some of these are unlikely to become available without concerted attention and directed resources. Others will become available much sooner, and provide a more powerful boost toward achieving major results, if they are developed systematically rather than emerging haphazardly. The Executive Committee refers to these enabling capabilities and facilities as the infrastructure for vadose zone S&T.

4.1 Generating and Compiling the Data for a Four-Dimensional GHCB Framework

All scientific endeavors require data to validate hypotheses, create models, and confirm or alter theories. For vadose zone science, data are also essential for developing and verifying simulations of past events and forecasting future conditions. Characterization and monitoring methods provide data that are crucial to understanding vadose zone processes, testing predictive models, and confirming performance of the site relative to regulatory and risk levels. Good data are essential for making good decisions about site remediation and long-term stewardship. Characterization of vadose zone processes and heterogeneities provides the data required to develop accurate simulations with the appropriate spatial resolution. Monitoring contaminant migration confirms the accuracy of simulations and can trigger remedial action.

In this section, the capabilities and infrastructure needed to generate these data and make them widely accessible are discussed under four headings:

- Virtual Library of GHCB Data,
- Sensors, Instrumentation, and Emplacement Techniques,
- Design and Optimization of Measurement Networks, and
- Field Facilities to Support Integrated Testing and Validation of Research.

4.1.1 Virtual Library of GHCB data

As explained in Section 2.1, the characterization and monitoring data for a contaminated vadose zone site must be adequate to provide a four-dimensional description (three spatial dimensions plus time) of the relevant processes and parameters in the vadose zone. A description of this kind depends on integrating measurement data and their interpretation across multiple traditional disciplines, including geology, hydrogeology, soil science, geochemistry, biology, geophysics, and geomechanics. In this roadmap study, an inclusive structure within which all these data types can be integrated is called a geological, hydrologic, chemical, and biological (GHCB) framework. Creating the four-dimensional descriptions for contaminated vadose zone sites will require concerted efforts to improve and create the tools and techniques to collect, qualify, correlate, and make accessible the data needed to implement a GHCB framework.

The focus for these efforts should be a GHCB virtual library, a virtual database of geological, hydrologic, chemical, and biological parameters as a function of geological environment. The GHCB virtual library could be implemented in several different ways. For example, it could be decentralized among a number of physical locations or more centralized. However implemented, it must be widely accessible to the communities engaged in research, site operations, regulatory oversight, and public involvement. It must accommodate multiple uses in characterization and monitoring activities, as well as provide a source of input data to numerical models for vadose zone system simulations.

The basics for a roadmap activity for creating a GHCB virtual library are highlighted in the following activity.

Activity G1. Build and extend a virtual library of qualified GHCB data.

- **Task with Near-Term Endpoint.** Tabulate known GHCB features for priority sites with vadose zone contamination and representative GHCB characteristics.
- **Near-Term Status Point.** GHCB virtual library is operational and contains qualified GHCB data for key sites with vadose zone contamination problems.
- **Near-Term Status Point.** Scale parameters are being reported to the GHCB virtual library, as well as measured values and distributions. Vadose zone scientists are comfortable interpreting their measured data using a hierarchical structure of organization that can exist in natural geological environments.

Quantitative GHCB models are populated using site-specific information. However, they are difficult to develop for unsaturated systems and require a significant investment in data collection, interpretation, and interpolation. Development is an iterative process in concert with numerical simulation of flow, transport, transformational processes, and data collection.

Activity G2. Develop prototypical numerical models that can be used to implement site-specific four-dimensional GHCB framework models incorporating site-relevant GHCB parameters and processes.

- **Mid-Term Status Point.** Prototype GHCB models are available that run with GHCB virtual library data and/or other suitably structured datasets.
- **Long-Term Status Point.** GHCB models and virtual library datasets are adequate to simulate the critical features, parameters and processes for the DOE vadose zone problem sites and other sites of national interest. The

simulations of flow and transport are consistent with all existing qualified data and observations.

Table 13 highlights major results that can be anticipated from the activities to develop a GHCB virtual library and quantitative GHCB models. The time horizons indicated in the table are contingent on sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under the activities.

Table 13 Highlights of Results for GHCB Data Library and Model Set Infrastructure Activities

	Near Term	Mid Term	Long Term
A virtual library of qualified GHCB data for priority contaminated sites is available to researchers, site operators, regulators, and the policy communities.	◆		
Virtual library data can be run on prototype models that incorporate a GHCB framework.		◆	
We can simulate critical features of priority contaminated vadose zone sites using GHCB models and virtual library data.			◆

4.1.2 Advances in Sensors, Instrumentation, and Emplacement

Limitations of Current Invasive Techniques. The nature of invasive vadose zone characterization and monitoring requires access to the subsurface through boreholes, trenches, or other excavations. While this direct access enables more direct characterization at many scales, it also has drawbacks, including:

- Problems of Access. Some contaminated sites contain high concentrations of chemical or radiological hazards that carry an exposure risk for workers involved in drilling or sampling at the site. Therefore the activities and movement of personnel and equipment must be carefully controlled and monitored to limit exposure.
- Effects on Flow and Contaminant Transport. Drilling, direct push, and other methods create new pathways for flow and contaminant migration.
- Effects of Sampling. The direct access methods directly perturb the soil and rock, therefore altering the processes and parameters of interest.
- Maintenance of Characterization and Monitoring Systems. Reliability of existing technology/instrumentation is an issue for monitoring over long time periods.
- Data Communications. Longer-term characterization and monitoring requires new approaches for communicating data from the subsurface and for minimizing or automating the data recording to selected intervals.
- Need for Improved Sensors. Over the next 25 years, there will be a revolution in sensor devices. The market for environmental restoration may not drive this new generation of sensor development. However, the environmental communities must find ways to influence the development of these sensors for new applications, so they can leverage the anticipated growth of this technology.

Research and development of new sensors, improved emplacement of new and current sensors, and novel emplacement approaches are key to enabling invasive characterization and monitoring. Also, research and development of new sampling methods for fluids, rocks, or soils are needed to reduce the effects of sampling disturbance and to reduce the impacts on the existing flow and transport system.

New Sensors. Over the next 25 years, there will a revolution in sensor devices. The advent of devices on the scale of microns and nanometers (microdevices and nanodevices) will generate opportunities for characterization and monitoring in the subsurface. These devices, along with advances in optical fiber sensors, will analyze chemical, biological, and flow processes. Examples currently appearing include "chemical laboratory on a chip" sensors and new geophysical sensors such as accelerometers. Microdevices will provide opportunities to gather data at more points per subsurface volume but at lower cost. New technologies for in-situ analysis of bioactivity will be continually developing over this period.

The market for environmental restoration may not drive the development of this new generation of sensors. However, to exploit the opportunities for leveraging these advances in sensor technology, the environmental communities must develop ways to direct the application of these sensors to subsurface characterization and monitoring of vadose zone (and groundwater) problem sites.

Improved Emplacement. In the near term, enhancements to instrumentation for existing technology, such as cone penetrometers, are needed. Gradually, between 2004 and 2025, new technologies such as microdrilling (1-inch diameter heads with their own coil tubing) are likely to find more application to vadose characterization and monitoring. Some of these technologies are already being developed for defense applications and fossil energy characterization. Microdrilling brings new capabilities in terms of size, cost, directional emplacement, and custom-composite tubing. Custom tubing can have built-in or attached microsensors and conduits for communication and sampling. In the longer term, autonomous drilling or miners, such as those developed for planetary probes (e.g., the Mars drilling program) and defense applications, will become available to address some emplacement needs in vadose zone characterization and monitoring. With these improved emplacement methods, new technologies for isolating boreholes and intrusions will be required.

Novel Emplacement Approaches. Over the next several decades, the vadose zone community must be prepared to adopt and adapt new and possibly revolutionary technologies as they emerge. For example, as sensors are miniaturized to micro and then nano scales, it may be possible to inject simple binary sensors that are pore size or smaller (similar in size to a colloidal particle) into soils or unconsolidated formations. These simple sensors could remain dormant until a chemical or environmental condition occurs, in response to which they emit a detectable signal. Other possibilities include miniaturized penetrators that can be shot into formations from boreholes, after which they would act as autonomous sensor packages.

Three roadmap activities to provide these capabilities are listed below. Table 14 highlights major results that can be anticipated from these activities, given sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under them.

Activity SIE1. Understand the effects of sensor emplacement and apply this understanding to improving sensor emplacement approaches.

- **Near-Term Status Point.** Methods for minimization of emplacement effects, such as microdrilling and coiled tubing, have been demonstrated successfully at important sites of vadose zone contamination, including DOE sites with high levels of radiological and chemical hazards.
- **Near-Term Status Point.** New drilling techniques for sampling and for sensor emplacement have been developed and tested.
- **Task with Mid-Term Endpoint.** Develop minimally invasive methods and approaches to correcting for emplacement effects.
- **Long-Term Status Point.** Non-invasive methods or methods to fully correct for emplacement effects are available for all characterization and monitoring needs.

For both characterization and monitoring, smaller sensor packages are of value for several reasons. If small, injectable sensors can fill in the data gaps between boreholes, they can increase the spatial density of data without the added cost and potential intrusion of adding more boreholes. For monitoring systems, even simple binary sensors can act as sentinel clouds in the vadose zone, triggering a response when a contaminant reaches them at a preset concentration or when a fluid pulse moves under a landfill cover. Small is also good because it enables mass manufacture, decreasing cost per sensor, making sensors disposable. Miniaturization also eases the implementation of multiple sensor types in one package.

Activity SIE2. Improve cost-effectiveness of sampling and sensor emplacement techniques.

- **Task with Near-Term Endpoint.** To decrease cost and improve spatial resolution, develop sensors that can fit in existing boreholes.
- **Near-Term Status Point**. Deployable prototype sensors are small enough that 10 sensors can fit inside a 2-inch diameter hole.
- **Mid-Term Status Point.** Cheaper, smaller, and more robust subsurface location devices have been developed and are available for use.
- **Mid-Term Status Point.** Prototype field sensors using alternatives to boreholes (cone penetrometers, new emplacements, microdrilling, autonomous devices, penetrators, injectable microdevices) are being deployed. These sensors are small enough to support 50 channels of output data in a sensor that fits in a hole the size of a rice grain.
- **Long-Term Status Point.** Injectable sensors and smart sensors are available as off-the-shelf technology. These low-cost sensor technologies provide

continuous spectrum coverage, are the size of a soil pore, and require little maintenance.

The following three status points apply to both Activities SIE1 and SIE2.

Near-Term Status Point (applies to Activities SIE1 and SIE2). The geology and hydrology of a contaminated site can be characterized at a 10-meter scale throughout the top 50 meters of the subsurface, using methods that have about a one-month turnaround time for processing and interpreting the field measurements.

Mid-Term Status Point (applies to Activities SIE1 and SIE2). The geology and hydrology of a contaminated site can be characterized at a 1-meter scale throughout the top 50 meters of the subsurface, using methods that have about a one-day turnaround time for processing and interpreting the field measurements.

Long-Term Status Point (applies to Activities SIE1 and SIE2). The geology and hydrology of a contaminated site can be characterized at a 1-meter scale throughout the top 50 meters of the subsurface in real time for most sites.

Table 14 Highlights of Results for Sensors, Instrumentation & Emplacement Infrastructure Activities

	Near Term	Mid Term	Long Term
Prototypes of miniaturized sensors are small enough to fit a package of 10 inside a two-inch hole.	◆		
We can characterize the geology and hydrology of a site at a 10-meter scale with one month turn-around.	◆		
Techniques to minimize emplacement effects have been developed and tested.	◆		
Minimally invasive emplacement methods and miniature sensors are available as alternatives to conventional boreholes and instrumentation techniques.		◆	
We can characterize the geology and hydrology of a site at 1-meter scale with a one day turn-around.		◆	
Injectable, smart sensors are available off the shelf; non-invasive methods for measuring key flow and transport properties are available.			◆
We can characterize the geology and hydrology of a site at 1-meter scale in real-time for most sites.			◆

4.1.3 Design and Optimization of Measurement Networks

Network Design

Subsurface characterization and monitoring for contaminants is difficult and expensive. Research in network design is needed to answer two significant questions: (1) How can we get the most information about subsurface contamination with the fewest boreholes, monitoring devices, etc.? (2) For compliance monitoring, how can we be sure that the vadose zone monitoring system will indeed detect if there is a leak of contaminants from an engineered waste disposal site?

Design approaches for monitoring networks, including kriging, pattern gridding, and others, aim for optimal placement of sampling points for detection monitoring at disposal sites. However, many of the models used for designing a compliance monitoring system have been developed for groundwater monitoring. Because of this regulatory emphasis on groundwater monitoring and the lack of requirements for vadose zone monitoring, vadose zone compliance monitoring has not had the sustained research focus needed to advance.

The state of practice needs to be reviewed in the area of subsurface monitoring system design. An optimization methodology for subsurface characterization needs to be developed that is based on flow and transport characteristics of the vadose zone at the disposal site. Finally, compliance monitoring designed to detect contaminant transport within the vadose zone should be encouraged. For sites where protection of valuable groundwater resources is an issue, it should be required.

Assessing the Value of Data

Vadose zone characterization and monitoring technology is evolving rapidly, presenting many options in developing and managing environmental sites for remediation or long-term stewardship. Among these options are "high tech" parameter-measurement approaches (e.g., three-dimensional and time-lapse three-dimensional geophysical surveys), novel emplacement methods, and advanced sensors. Today's environmental management team must be able to use new technologies and methods that have been designed to provide better and more accurate information about the site in question. At present, however, there are no objective means to evaluate environmental technologies. Research should be focused on developing a system (e.g., a decision support system) with which environmental managers can readily and rapidly prioritize locations for characterization and monitoring activity and allocate discipline-specific expertise and other resources.

The following roadmap activity incorporates research needed to design optimal monitoring networks for the vadose zone and assess the value of environmental characterization and monitoring technologies relative to site-specific objectives. Table 15 highlights major results that can be anticipated from this activity, given sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under it. The role of numerical laboratories, mentioned in Activity ND1, is discussed in the next section, on facilities for integrated field experiments.

Activity ND1. Develop, test, and apply methods for optimizing vadose zone sensor networks to meet end users' needs for characterization, site-wide assessment, and monitoring information within user-specified constraints of uncertainty and cost.

- **Task with Near-Term Endpoint.** Create a numerical laboratory, combined with highly instrumented field sites, for assessing sensor networks and data value. Define numerical experiments to assess the value of data.

- **Task with Near-Term Endpoint.** Develop methods to determine the sensitivity of key parameters to sensor network design (and indirectly, cost).
- **Task with Near-Term Endpoint.** Determine how design and optimization of sensor networks can reduce uncertainty, taking into account the factors of sensor network cost, data density, and subsurface depth.
- **Mid-Term Status Point.** The numerical laboratory has been upgraded and can now be combined with field data to apply methods for network sensor design to field-scale tests and experiments.
- **Task with Mid-Term Endpoint.** Develop methods to identify controlling parameters.
- **Mid-Term Status Point.** The geophysical method or combination of methods that is most cost-effective for characterizing different geological environments or dynamic processes can be determined.
- **Long-Term Status Point.** Sensitivity to network design can be quickly determined for complex-wide sites.
- **Long-Term Status Point.** Network design and optimization methods are used to convey to end users the cost, data density, and level of investment needed to reduce uncertainty to specific levels.

Table 15 Highlights of Results for Design & Optimization of Measurement Networks Infrastructure Activities

	Near Term	Mid Term	Long Term
We can access a numerical laboratory linked with instrumented field sites to conduct experiments on characterization/monitoring network design and data value.	◆		
We can use field data in a numerical laboratory to optimize monitoring networks for field-scale experiments.		◆	
We can use network optimization design methods to explain cost-benefit risks and other trade-offs to end users, as part of planning for long-term monitoring and site assessment activities.			◆
We can quickly determine the location sensitivity and data value for designs of monitoring and characterization networks.			◆

4.2 Field Facilities to Support Integrated Testing and Validation of Research

A number of the research activities presented in Sections 2 and 3 specify integrated field experiments (IFEs) as the means to achieve important results.[14] This section describes the kinds of facilities required for these experiments. It also explains why the facilities and the IFEs are crucial to achieving many of the mid-term and long-term results of research described elsewhere in this roadmap.

[14] See Activity PH2; Activity CH4, long-term status point; Activity SC1, mid-term task for hierarchically scaled flow and transport models; and Activities IV1 through IV4.

4.2.1 The Role of Field Experiments in an Integrated Approach to the Vadose Zone

A central theme of this roadmap is the importance of providing an integrated four-dimensional data framework and site-specific models for the vadose zone. This integration must incorporate process knowledge and site-specific data from across traditional disciplines. Important requirements for this integration include the capability to determine the relevant parameters to be measured at site-specific locations and the capability to select characterization and monitoring methods (including frequency of measurement) optimized for those locations. As part of determining the value of data, capabilities are needed to compare the cost with the benefit of additional data, including the precision required, for specific parameters and locations. When a lack of data or process understanding leaves doubts about the best process representation, well designed and controlled field experiments can discriminate between alternative conceptual models crucial to building a successful site-wide model.

Multidisciplinary field experiments, if focused on answering specific questions or hypotheses regarding vadose zone processes, provide a means for testing and validating both the components being integrated and the integration methodology. However, to test the data framework and models, the experiments must be run in a reasonably well characterized environment, so that test results can be compared against a validated "ground truth" for that site. Thus, to get the most value from IFEs, they should be conducted at sites whose GHCB characteristics are reasonably well known and can be monitored during the course of the experiment.

After the model representations, site-specific boundary conditions and parameters, and the monitoring network have been validated through an IFE, the resulting integrated model can be extrapolated forward in time to assess the risks associated with impacts on groundwater and other routes for environmental and health exposures. Scenarios can be run to examine remediation alternatives, such as the impact on contaminant transport if an engineered barrier is placed over subsurface waste.

In these experiments, "everything comes together." IFEs conducted at suitable sites will allow a broad range of hypotheses to be tested and tentative results (from laboratory, small field-scale, or computer-based research) to be assessed (disconfirmed or validated). An infrastructure of facilities for conducting IFEs would bring together and amplify much of the research described in Sections 2 and 3. It would also complement other elements of infrastructure, such as the GHCB virtual library and the vadose zone Problem Solving Environment, described elsewhere in Section 4. Among the many *kinds* of research questions and results amenable to exploration with well-designed IFEs are the following:

- New sensing technologies, both invasive and non-invasive;
- Monitoring and characterization strategies and techniques, including sensor network design and optimization for environments similar to the test site;
- Conceptual models that represent hypotheses about underlying processes and properties, as well as coupling of processes in specific conditions and subsurface environments; and
- Site-wide integrated models incorporating multiple process models and running with GHCB boundary data derived from characterization studies and monitoring networks for that site.

For example, an IFE could be set up as a scenario that may occur during cleanup of a contaminated site, such as discovery of a previously unknown waste burial ground. The experiment's objectives would include characterizing what is leaking and how fast it is moving horizontally and vertically in the vadose zone, predicting where it will go, and establishing an appropriate monitoring network. The experiment would be set up with known boundary conditions based on prior characterization of the site. In addition to gathering data from both existing and newly installed monitoring networks, the experimental design might include subsurface sampling to verify or calibrate sensor data.

IFE facilities and sites should be selected and established with the understanding that long-term (continuing a decade and longer) experiments will be conducted, as well as shorter-term experiments. Long-term IFEs are essential for testing and validating both process understanding and integrated site-wide models at multiple spatial and temporal scales. The facilities should be established and operated to provide opportunities for iterative work. Once these experiments are started, unexpected results will occur for which more data or different kinds of data will be needed to test, refine, and validate hypotheses, models, and the understanding derived from interim results.

An important aspect of IFE design should be a multidisciplinary approach. Research scientists and technology developers (including technology users) from different disciplines and work interests should participate in designing, installing, conducting, and analyzing the results from an IFE. Establishing a number of sites for such tests would contribute to an integrating environment for researchers and practitioners who too often have worked in isolation.

Sites where long-term, integrated experiments can be conducted are essential for bringing together researchers from different disciplines in a team approach. In the process of designing and conducting IFEs, expertise from multiple disciplines is needed. During each experiment, much will undoubtedly be learned about the physical, chemical, and biological processes occurring in the subsurface. Thus, IFEs can be a real integrator, moving researchers and practitioners toward the goal of thinking and working within an integrated GHCB framework.

To ensure that these larger purposes are achieved, operations at the IFE facilities must bring together researchers and practitioners from across disciplines for the design, conduct, and interpretation of the IFEs. The objective should be to create a cross-disciplinary "think-tank" environment. The long-term IFEs, in particular, should be set up to force interdisciplinary teaming.

4.2.2 Facility Requirements for IFEs

To test models for predicting the field-scale fate and transport of contaminants in the vadose zone, facilities will be needed to conduct appropriate experiments and investigations. These same facilities may also be used to test and evaluate tools and techniques for characterizing and monitoring contaminant behavior. The type of experiments needed to yield a better fundamental understanding of vadose zone processes will depend on the phenomena being investigated. In some cases, smaller experiments will suffice; however, larger experiments will likely be necessary to investigate vadose zone system behavior relevant to major contaminated sites. The larger experiments may start with laboratory modeling, using a numerical laboratory as described below. The advantage of this preliminary step is that it allows rigorous evaluation in controlled conditions of conceptual models, sensor network design, and other critical experimental parameters before proceeding to the field experiment. Therefore, the type of facilities needed to support research outlined in this roadmap range from small bench-top equipment to specialized laboratory facilities to instrumented, well-characterized field sites.

Currently, most universities and national laboratories have facilities for conducting small-scale experiments. Relevant subsurface phenomena may be studied using these facilities under highly controlled conditions. However, it is unlikely that the research results can be used to verify consequences of field-scale contaminant behavior. The research conducted with these small-scale facilities will generally need to be coupled with research conducted at a larger-scale before being applied in the field.

4.2.3 Relationship between Laboratory Capabilities and IFE sites

As noted in Section 3.4, computer-based synthetic test problems are one element in an integrated approach to testing and validating models. A computer-based "numeric laboratory" can also provide an initial assessment for testing and optimizing the design of a sensor network for initial site characterization or continuing monitoring. One or more numerical laboratories equipped for simulating proposed IFEs would therefore complement development of sites and facilities for the subsequent experiments in the field. Ideally the numerical laboratory would allow for modeling of the sensor network and placement strategy for the IFE, as well as providing synthetic test cases for the models to be used, covering several scenarios relevant to the experimental context and hypothesis.

Specialized facilities are also needed in which to conduct large experiments (up to 2,000 cubic meters in size) relevant to the needs of major contamination sites, such as some DOE and other national priority sites. An advantage of conducting large experiments in specialized facilities is that they can be more controlled than field experiments while allowing field-scale phenomena to be studied. Boundary conditions can be controlled to investigate specific phenomena and to observe responses to environmental changes more quickly than can be observed in field experiments. Properties can be engineered to reflect heterogeneous field conditions, which will allow better interpretation of the experimental results because the properties will be known in greater detail than for field experiments. Physical, chemical, and biological measurements will be easier to conduct because there will be greater access to the experimental domain than in field experiments.

The large experiments can be designed to help distinguish between alternative field-based conceptual models of subsurface contaminant behavior, evaluate the long-term performance of subsurface-engineered solutions, and conduct prototype and proof-of-principle testing before field application. Other important aspects of large experiments in specialized facilities are that ‘real’ contaminants (e.g., chemical and radioactive hazards and biopathogens), which could never be released in the field, can be studied under controlled conditions. The large-experiment facilities will be a resource for conducting field-relevant, multidisciplinary experiments that will bring together the best technical minds with state-of-science research tools.

4.2.4 An Approach for Initiating Development of IFE Support Facilities

To begin development of IFE support facilities, representative field sites designated for such experiments must be established. They will be most useful if located in the most representative subsurface conditions where serious contamination problems are being addressed. To take just DOE’s vadose zone contamination problems as an illustration, an initial set of sites might include: (1) macroporous strata such as are found at the Hanford Site; (2) fractured rock like that at Los Alamos, the Yucca Mountain Project, or parts of the Nevada Test Site; and (3) sandy strata in climates with higher annual recharge, such as the Savannah River Site. This set should be expanded or adjusted to cover representative vadose zone conditions that are priorities for agricultural contamination (e.g., sites typical of hyper-salinization and of subsurface transport of agricultural chemicals or pathogens), burial sites and firing ranges on military reservations, and other subsurface conditions represented by sites on national priority lists. Obviously, the key federal (and state) agencies involved, including the Departments of Agriculture, Defense, and Energy, as well as the Environmental Protection Agency, the U.S. Geological Survey, and state environmental and public health entities, should work together to draw up a short list of the best sites to meet the most pressing needs.

A key requirement for all the selected sites is that they remain stable and accessible for several decades after the IFE facility is established. After a site has been designated for an IFE facility, there would be a call for a research coordinator to organize, coordinate, and conduct the experiments at the facility. The experiment and the process should be structured to bring together geologists, geochemists, hydrologists, biologists, and others in both the design and interpretation of experiments.

Activity IFE1. Select, develop, and use national facilities for integrated field experiments aimed at testing vadose zone research and technology.

- **Near-Term Task**. Design and construct IFE support facilities at one or (preferably) more sites representative of priority vadose zone contamination conditions.
- **Mid-Term Status Point.** A first series of shorter-term experiments have been completed.
- **Long-Term Task.** Conduct major, long-term integrated field experiments (designed to continue for a decade and longer).

Table 16 highlights major results that can be anticipated from this activity, given sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under it.

Table 16 Highlights of Results for Facilities for Integrated Field Experiments Infrastructure Activities

	Near Term	Mid Term	Long Term
Facilities to support IFEs have been constructed at representative sites.	◆		
Results from the first series of short-term IFEs are available.		◆	
Results from major, long-term IFEs are supporting and testing long-term research efforts, improving monitoring systems, and validating integrated assessment models.			◆

4.3 Computational Resources to Develop Adequate Models and Simulation Capabilities

Models are most often thought of as predictive tools for making useful and cost effective estimates of future conditions or, sometimes, reconstructions of past events. Models can be used to explore alternative design and operational decisions for characterization, monitoring, and remediation, as well as to compare and contrast policy options such as remediation and long term stewardship.

Modeling is essential to understanding subsurface environments because these environments are inherently complex, difficult to access, and therefore incompletely understood. They exhibit a diverse set of important phenomena on a wide range of temporal and spatial scales. They are heterogeneous and difficult to characterize and monitor. For these reasons, models of vadose zone systems serve a much more fundamental purpose than being a tool for prediction or reconstruction. They are used to synthesize and integrate our understanding of basic processes, particularly the coupling among processes across spatial and temporal scales. Models built for application at a specific site may have more value in this synthesizing role than they do in making predictions. The synthesis can be informal and ad hoc, or it can be based on formal inversion algorithms and married to both characterization and monitoring data.

Predictive and inversion models of vadose zone systems are based on numerical methods. The resulting computer simulation models only have value if they are pertinent to questions being asked by decision makers, accurately reflect the vadose zone system being modeled, and are obtained in a timely manner. The research identified and discussed in this section is aimed specifically at these numerical models and has been organized to address two important criteria for successful modeling: productivity and predictability.

The usefulness of model results is directly related to the time it takes to build a model, produce a computer simulation, run an inversion, or even display the visualization. To improve the usefulness of models, one can ask, “What new simulation/visualization tools are needed to improve user productivity?” That is, what do the site investigator, the decision-maker, or the researcher need to make better use of their time and resources? These productivity questions are answered by research in three areas: modern software; hardware; and mathematical algorithms, all designed specifically for vadose zone applications. These three areas are discussed in the remainder of this section.

The second criterion for models addresses the question “What features and capabilities must vadose zone modeling tools possess to both maximize and measure predictability?” The answer to this question involves all of the GHCB processes discussed earlier. Particularly important, and difficult, are challenges in how modeling tools treat coupled GHCB systems, scaling, and uncertainty. Research needs in these areas are described in Section 3.1, as well as in the discussion of model integration and validation in Section 3.4. Improvements in software; hardware; and mathematical algorithms, discussed below, will also improve predictability, in part by allowing the research results developed through Section 2 and 3 activities to be applied in integrated vadose zone simulations.

4.3.1 The Problem Solving Environment: Integration of Data, Knowledge, and Models and Generalization to Other Sites

There are a large number of possible conceptual and mathematical models applicable to vadose zone GHCB systems. The number of numerical approximation methods and visualization tools is also large, and growing. This sign of maturity aside, modeling of any complex subsurface system is a difficult task, which often leads to compromises in adequacy of the model or numerics used for a particular application. Further, implementing a new model for a complex subsurface system can take months to years of effort, yet new models are needed routinely for sites where wastes have been buried or released to the ground by other means.

User interfaces for many modeling applications are crude and inflexible. Often, several different computer programs must be inefficiently linked together. The data are typically available only in diverse and incompatible formats. The effort required to interpret results from one application to the next strains human and budgetary resources. It also consumes time before the model can be run to produce useful output. Consequently, corners are often cut, especially at the research level where most computer software is developed. These constraints have led to a large number of limited-use computer programs, each of which is used—and improved—by only a small number of people. In many cases, only the developer understands the strengths and limitations of a modeling tool well enough to use it efficiently and appropriately.

These problems can be resolved through the development of a friendly and usable *vadose zone problem solving environment* (PSE). In formal terms, a PSE is an integrated software framework that provides the functionality needed for a complex set of tasks, accessible through an efficient, high-level interface. Mathematica© and MATLAB© are examples of commercially available PSEs. However, for a variety of reasons these and other commercial products are not suited to the task of building integrated system models for vadose zone environments. A vadose zone PSE should unify mathematical, scientific, and engineering concepts and constructs in a single framework. It should allow for rapid set-up of problem specifications and easy manipulation and visualization of data.

The development of a PSE for modeling and visualizing subsurface systems, while quite challenging, would significantly enhance productivity for those developing, improving, or applying models, as well as those relying on model output for decision support. It would encourage a greater number of hypotheses to be tested and decision variables to be quantified than is currently possible, inspiring greater confidence in the model outputs and the decisions based on them. It could and should be integrated with related characterization and monitoring tools. (A number of these potential tools for integration are listed in other roadmap activities).

The following two roadmap activities outline the work and time frame required to implement a first-generation vadose zone PSE, as well as the R&D needed to extend and improve it incrementally through subsequent software generations. Table 17 highlights major results that can be anticipated from these activities, given sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under them.

Activity PSE1 (near-term). Develop and implement a useful first-generation vadose zone PSE.

- **Task with Near-Term Endpoint** (subtask of PSE1). Develop the basic PSE structure, including a high-level interface, data structure storage and retrieval approach, simulation engine, and graphical back-end, with a common data structure for modeling and characterization/monitoring.
- **Task with Near-Term Endpoint** (subtask of PSE1). Implement a limited set of state-of-the-art numerical methods for the first-generation PSE.
- **Near-Term Status Point.** A first-generation PSE is implemented, functional, and in use. This version is likely to have the following characteristics: (1) restricted to structured grids, (2) implemented on workstations, (3) implemented for forward simulations, and (4) applicable on a limited basis to the real-world problems of sites with vadose zone contamination.

Activity PSE2. Extend and update the vadose zone PSE to provide an increasingly powerful and integrated software framework for studying and solving problems in vadose zone contamination.

- **Mid-Term Status Point.** Location-specific databases of parameters have been built and populated.
- **Mid-Term Status Point.** The PSE has matured to provide users with a wide range of models, including some multi-scale, coupled models.
- **Mid-Term Status Point** (also a status point for Activity CP2, in Section 3.1.2). Models for strongly coupled nonlinear GHCB systems are supported in the vadose zone PSE.
- **Mid-Term Status Point** (also a status point for Activity IV2 in Section 3.4). A computational test bed to assist in testing and validating models has been incorporated into the vadose zone PSE.
- **Mid-Term Status Point** (also a status point for Activity IV2 in Section 3.4). Support for inverse methods and for decision support simulations has been added to the vadose zone PSE.
- **Mid-Term Status Point** (also a status point for Activity IV2 in Section 3.4). Geographical information systems have been linked with, or otherwise functionally incorporated into, the vadose zone PSE.
- **Mid-Term Status Point** (related to a task and several status points for Activity UC3 in Section 3.3). Support for uncertainty analyses has been incorporated into the vadose zone PSE.
- **Mid-Term Status Point** (also a crosscutting status point for numerics R&D activities in Section 4.3.2). Support for a wide range of numerical methods has been incorporated into the PSE.
- **Mid-Term Status Point.** The vadose zone PSE has been implemented on state-of-the-art supercomputing environments.
- **Mid-Term Status Point.** The vadose zone PSE is being used routinely by DOE and other agencies for visualization, analysis, and simulations in support of characterization, monitoring, site assessment, and remediation/stewardship decisions at major sites of vadose zone contamination.
- **Long-Term Status Point** (also a crosscutting status point for Activities CP1–CP3 in Section 3.1). Realistic models for all coupled GHCB phenomena, including strongly coupled nonlinear processes, that are important to vadose zone flow and transport are available in the PSE. These models cover all important time and space scales.
- **Long-Term Status Point.** The vadose zone PSE supports state-of-the-art numerics, including full spatial and temporal error estimation with automatic grid refinement.

- **Long-Term Status Point.** Support for assessing the value of information has been added to the vadose zone PSE, including the Shared Vadose Model (described in section 3.4).
- **Long-Term Status Point.** The vadose zone PSE is broadly accepted and used as a valuable tool to assist all aspects of the development and application of the science: processes, characterization and monitoring, simulation, and prediction.

Table 17 Highlights of Results for The Problem Solving Environment Infrastructure Activities

	Near Term	Mid Term	Long Term
We can access a shared PSE (software), which includes a common data structure for use in characterization, monitoring, and modeling, as well as a limited set of numerical modeling tools.	◆		
An extended PSE, linked to a geographical information system, incorporates a range of numerical methods and provides a computational test bed for validating models.		◆	
The vadose zone PSE incorporates realistic models for all coupled GHCB phenomena and state-of-the-art numerics; it supports 'value of information' assessment for monitoring and characterization systems.			◆

4.3.2 Advanced Numerical Algorithms

Although advances in computer hardware will aid the modeling effort, they cannot provide all of the necessary improvements in light of issues like scaling and extreme gradients. Furthermore, the usefulness of model results is directly related not only to the time required to produce a simulation but also to the confidence that a decision-maker can place on the results. The simulation should be accurate, and it should provide some quantified indicators (metrics) for the likely range and probability of numerical error.

4.3.2.1 Adapting Advances in Numerics to Vadose Zone Modeling

Ongoing basic research on linear and nonlinear solvers, optimization techniques, grid generation, parallel computing techniques, visualization, and other areas can have a large impact on vadose zone simulation. However, these general advances in numerical algorithms (numerics) must first be adapted to the particular needs and resources of vadose zone simulation. In particular, existing state-of-the-art linear and nonlinear solution techniques need to be adapted to vadose zone simulation, including the development of appropriate preconditioners and multilevel techniques. To capture meaningful space and time scales of important GHCB phenomena, especially non-continuum and chaotic phenomena, new and sophisticated multi-scale numerics are required.

Activity NM1. Development and application of better linear and nonlinear solvers to vadose zone modeling.

- **Near-Term Status Point.** Existing state-of-the-art linear and nonlinear solvers have been adapted, improved, and applied to vadose zone problems.

- **Mid-Term Status Point.** Linear and nonlinear solvers have been improved to match vadose zone problems and run in computing environments, such as the vadose zone PSE.

Activity NM2. Improve approaches to resolve extreme spatial gradients in GHCB properties and processes, such as fingers, sharp fronts, boundaries, and interfaces.

- **Near-Term Status Point.** State-of-the-art numerical methods are being applied to modeling spatial gradients of fingers, sharp fronts, boundaries, interfaces, and other extreme-gradient GHCB phenomena.
- **Mid-Term Status Point.** New and improved numerical methods have been developed and applied for resolving extreme GHCB gradients in both space and time.

Activity NM3. Develop multi-scale mathematical methods and numerics to capture meaningful scales of important GHCB phenomena.

- **Mid-Term Status Point.** Multi-scale mathematical methods and numerics are in use for modeling important GHCB processes, including most linearly coupled, continuous processes.
- **Long-Term Status Point.** More sophisticated multi-scale mathematical modeling and numerics have been developed, targeted to non-continuum and chaotic phenomena.

4.3.2.2 Error Estimation Numerics

Sources of numerical error in computer simulations have many origins. Simulating evolving processes in spatially and temporally discrete increments is one widely recognized source of numerical modeling error. Refining spatial grids and time steps can reduce these errors. However, in heterogeneous systems like those typical in the vadose zone, refinement is needed only in certain regions of space and/or time. To save computational effort, the computation should automatically and adaptively refine its grid and/or time steps locally, as necessary to maintain accuracy. For the same reason, it should, if possible, adjust the amount of source detail required.

Time truncation error is particularly difficult to estimate and control. It accumulates from one time step to another, and is often self re-enforcing (i.e., it exhibits positive feedback). However, there are limits to refinement, even aside from computational resource issues. As refinement increases, so does rounding error and ill conditioning of the system.

Certain types of algorithms contribute other numerical artifacts, such as numerical instability, nonconservation of mass, violation of the maximum principle (i.e., creation of nonphysical local maxima or minima in the solution), numerical dispersion, and initiation or non-initiation of physically relevant frontal instabilities. Such errors are often not ameliorated by refined grids and reduced time step intervals because the mathematical structure itself is improperly approximated. Of particular interest is the ability to resolve features such as extreme spatial and temporal gradients without producing numerical oscillations. These issues must be investigated and resolved within the context of vadose zone applications.

Activity NM4. Develop and apply spatial numerical error estimators and adaptive local (spatial) grid refinement algorithms.

- **Near-Term Status Point.** Numerical errors are being estimated in terms of quantities of interest to decision-makers, using spatial numerical error estimators and adaptive, spatially local, algorithms for grid refinement.

Activity NM5. Develop and apply spatial and temporal error estimators and adaptive local grid and time step refinement algorithms for nonreactive systems.

- **Mid-Term Status Point.** Both spatial and temporal error estimators and grid refinement algorithms (for spatial grid and time steps) are being incorporated in nonreactive flow-and-transport models.
- **Long-Term Status Point.** Spatial and temporal error estimators and adaptive local grid and time step refinement have been developed and are being applied for reactive systems in the vadose zone.

4.3.2.3 Warning or Protecting Users from Modeling Errors and Constraints

Beyond improving numerics to reduce modeling error, algorithms are needed that automatically alert the user to a model's possible numerical limitations through quantified error range estimates. An even more significant development would be algorithms that self-adaptively select a more accurate alternative approach. Numerical error estimates should also be expressed in measures of interest to decision makers.

For example, estimation of decision variables (mathematically referred to as functionals of the solution) and their variance is more meaningful than merely trying to estimate the norm of the global error. A functional can be overly sensitive to small errors in the solution or data at some point in time and/or space, even though the global error appears to be quite small. Conversely, the functional may be insensitive to such errors, therefore reducing computational effort. Useful algorithms must not only estimate the mean and variance of quantities of interest to a decision maker, but also provide information on the likely error in those quantities generated from a variety of sources, including numerical resolution, inadequate or inappropriate numerics, scaling, and noisy data. These numerical algorithms should be used together with algorithms tracing uncertainty due to the conceptual model, uncertain and variable parameters, initial conditions, and boundary conditions.

The envisioned algorithms must be ported to the vadose zone PSE, discussed in Section 4.3.1, or their enormous complexity would limit their utility to practitioners and regulators who are not well versed in numerical techniques and computational issues.

Activity NM6. Determine criteria for acceptable computational errors based on model uncertainties and incorporate algorithms for these criteria in vadose zone simulation software.

- **Mid-Term Status Point.** Probabilistic approaches to estimate likely numerical error are available for use in vadose zone system modeling, instead of maximum error. These probability approaches are being used to estimate mean and variance, as well as other numerical error measures, in terms of quantities of interest to decision makers.
- **Long-Term Status Point.** Estimates of maximum, mean, variance, and other numerical error measures in quantities of interest to decision makers are standard practice in modeling vadose zone systems. Modelers use these estimates adaptively to improve simulation results.

The following status points apply to all of Activities NM1 through NM6. Table 18 highlights major results that can be anticipated from these activities, given sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under them.

Mid-Term Status Point (applies to Activities NM1–NM6; also a status point for the vadose zone PSE in Section 4.3.1). Support for a wide range of numerical methods has been incorporated in the vadose zone PSE.

Long-Term Status Point (applies to Activities NM1–NM6). In models of vadose zone systems, the numerical methods are selected automatically and on an appropriate scale, during computation, to reduce numerical error in decision variables.

Table 18 Highlights of Results for Advanced Numerical Algorithms Infrastructure Activities

	Near Term	Mid Term	Long Term
Existing state-of-the-art numerical methods have been adapted to address vadose zone problems.	◆		
A wide range of numerical methods relevant to vadose zone problems are available.		◆	
Site assessment models can automatically select the best numerical method at a spatial and temporal scale to minimize numerical error in decision variables.			◆

4.3.3 Computing Power: A Dedicated, High-Powered Capability

Sheer numerical speed addresses both productivity and predictability. Vadose zone simulations must resolve extreme spatial and temporal gradients, capture multi-scale coupled processes, and handle large data sets. Uncertainty analyses dramatically increase the load on computational resources.

Today, almost everything is done on fast desktop machines or networked high-end workstations. Nevertheless, the computing and storage memory capacities of these systems, as well as their processor, bus, and network speeds, limit their capacity to represent vadose zone processes realistically, synthesize data, compute forward predictions, or visualize information. Occasionally simulations are run on teraflop machines (processors capable of performing a trillion basic arithmetic operations per second), such as the Accelerated Strategic Computing Initiative's (ASCI) Blue and White Machines. But access is limited due to competing high-priority uses and tight security precautions. In short, the present generation of hardware available to the vadose zone R&D community is inadequate.

The vadose zone community needs priority access to state-of-the-art massively parallel computers, like the ASCI's teraflop machines. The vadose zone community would use these machines for research into multi-scale processes and process coupling, for characterization, for modeling and prediction, and for visualization. The machines could be housed at one or more national laboratories. Priority use could be given to researchers from universities and the national laboratories who are working on a range of environmental science and technology issues, not just the vadose zone.

Such a facility would require a dedicated computer support staff to help environmental scientists and engineers prepare their computer programs for parallel processing and port them to the massively parallel computer. This staff could also unite these new computation resources with the proposed vadose zone PSE. The support staff could be patterned after the staff that runs the ASCI Blue and White machines, at the Center for Applied Scientific Computing at Lawrence Livermore National Laboratory.

Activity HPC1. Design, implement, and continue to improve an Environmental Science High-Power Computing capability.

- **Task with Near-Term Endpoint.** Build a user community; form an organizing committee.
- **Task with Near-Term Endpoint**. Write the proposal for a multi-teraflop (10^{13} to 10^{14} Flops) computing capability, to be associated with the DOE Environmental Management Program and/or the Office of Science.
- **Near-Term Status Point**. Proposal for a multi-teraflop computing capability has been submitted to DOE.
- **Near-Term Status Point.** Design of the computing capability has been completed, including its expected future growth in size and capability.
- **Task Beginning after Above Status Points, Completed in Mid-Term.** Purchase and install the computing capability at a national laboratory; hire staff.
- **Mid-Term Status Point.** A high-power computing capability is in use by a large variety of vadose zone researchers on studies of processes, characterization/monitoring, and modeling. It is used to study both laboratory and field experiments. It is also being used in applied studies for environmental management sites by DOE and other "problem holders."

- **Task beginning in Mid-Term with Mid-Term Endpoint.** Form a committee and write a proposal for the next generation of computing capability.
- **Mid-Term to Long-Term Status Points.** The next-generation computing capability is designed, purchased, and installed.
- **Long-Term Status Point.** A next-generation high-power computing capability is in common use for addressing vadose zone problems.

Activity HPC2. Build (or transfer from ASCI and others) infrastructure such as desktop visualization, archival storage, and parallel input/output interfaces.

Activity HPC3. Train the user community for the environmental science high-power computing capability.

Activity HPC4. Port the vadose zone PSE to run on the environmental science high-power computing capability.

Table 19 highlights major results that can be anticipated from these infrastructure development activities, given sufficient support and programmatic direction to accomplish the detailed tasks and achieve the status points listed under them.

Table 19 Highlights of Results from High-Powered Computing Infrastructure Activities

	Near Term	Mid Term	Long Term
A proposal is submitted to DOE and acquisition of the EHPCC begins.	◆		
First generation EHPCC is in use.		◆	
Second generation EHPCC is in use.			◆

5.0 CONCLUSIONS AND RECOMMENDATIONS

The technical content of the Vadose Zone Science and Technology Roadmap consists of the activities presented in Sections 2 through 4. (Appendix B shows all the roadmap activities, with their associated tasks and status points.) This section provides concluding reflections on these activities when viewed as a whole. It also contains suggestions from the Roadmap Executive Committee on how best to understand, prepare for, and sustain the activities *as a roadmap for addressing issues of national importance.* The Committee has provided additional suggestions on a path forward for following, expanding, and updating the roadmap in a separate document, *Letter Report of the Vadose Zone S&T Roadmap Executive Committee on Creation of a National Multi-agency Vadose Zone Science and Technology Initiative*.

5.1 The Bottom Line: Highlights of Expected Results from Roadmap Activities

Table 20 presents the results that have been highlighted at the close of previous sections as useful outcomes of the roadmap activities. These highlights have been selected (and worded) to convey to a broader, nontechnical audience how the public and the nation will benefit from investing in vadose zone research (i.e., the bottom line). Readers with an interest in technical detail and context should consult the activities and the accompanying narrative in Sections 2 through 4.

The highlighted results are keyed to the same time horizons used for the roadmap activities. *Near-term* means roughly within 4 years of beginning roadmap implementation. *Mid-term* means the results can be expected within a decade or so. *Long-term* applies to results over several decades (roughly, a 25-year horizon). These time horizons, as noted earlier, depend on sufficient resources and programmatic direction being applied, at the right time and place, to accomplish the tasks and reach the status points detailed in the roadmap. Table 20 provides a convenient way to survey the results by time horizon, to consider what can be achieved quickly, what will take more than a few years, and what will require sustained effort over several decades.

Table 20 Highlights of Expected Results from Roadmap Activities

	Near Term	Mid Term	Long Term
#1 Physical Description of Flow & Transport			
Computer models used by federal agencies and others incorporate the best state-of-the-art conceptual models and implementations (software modules).	◆		
We can detect the presence of fluid in fractures in some cases.	◆		
We can distinguish, in most cases, the subset of fractures that are conduits for fluid flow and contaminant transport.		◆	
We can map and predict water distribution and flow through structured soils or fractured rock at multiple spatial scales.		◆	
Monitoring data on fluid flow and contaminant transport can be interpreted and represented visually at site-wide scales in real-time.			◆

Table 20 Highlights of Expected Results from Roadmap Activities (cont.)

	Near Term	Mid Term	Long Term
#2 Chemical Properties & Processes			
Reaction kinetics and rate laws (in solution) have been formulated for priority vadose zone conditions.	◆		
Individual chemical contaminants in the vadose zone can be detected.	◆		
We understand the kinetics for important chemical reactions at solid and liquid interfaces (e.g., ion exchange and colloids) in vadose zone conditions.		◆	
Flow and transport models map and predict important vadose zone chemical interactions, including those involving mixtures of solids, liquids, and air.			◆
#3 Biological Properties & Processes			
We understand and can predict how microbial processes affect or are affected by bioavailability of important contaminants.	◆		
We can measure biochemical rates, in situ bioavailability, and the composition and activity of microbiological communities.	◆		
Reactive transport models can predict how microorganisms will interact with contaminants.		◆	
Inexpensive systems are available to measure community composition and activity.		◆	
We can accurately predict site-specific biodegradation rates for important contaminants.			◆
We can take biological measurements along with others without destroying the samples.			◆
#4 Colloidal Formation & Transport			
We know how to detect mobile colloids and how to sample and analyze them.	◆		
Important colloid-contaminant interactions understood at micro and macro levels.		◆	
Flow and transport models can map and predict important colloidal interactions and transport.			◆
#5 Multiphase Flow & Transport			
We can model processes with unstable or preferential flow of aqueous and non-aqueous phases.	◆		
We can detect and interpret multiphase flow and transport of complex contaminant mixtures at contaminated sites.		◆	
Site assessment models incorporate multiphase flow and transport.			◆
#6 Unstable Processes			
We can identify the onset of chaotic and unstable processes.	◆		
We can determine whether and when chaotic conditions are important at a site.		◆	
Site assessment models incorporate models for chaotic and unstable flow.			◆
#7 Understanding and Modeling Coupled Systems			
The highest priority coupled GHCB processes have been identified.	◆		
We understand the strengths and weaknesses of existing models.	◆		
Some of the important strongly coupled phenomena can be modeled.	◆		
Process models for important strongly coupled phenomena have been validated and field-tested across spatial and temporal scales.		◆	
Site assessment models incorporate all important coupled GHCB phenomena realistically.			◆
#8 Combining Processes & Data at Different Scales			
We can simulate scaling problems of important GHCB phenomena using probabilistic modeling.	◆		
We can measure and model coupled GHCB phenomena across spatial scales.		◆	
Site models incorporate strongly transient and coupled GHCB phenomena for multiple time periods.			◆
Site models incorporate scaling with estimates of uncertainty, and the models can propagate uncertainty estimates across spatial and temporal scales.			◆

Table 20 Highlights of Expected Results from Roadmap Activities (cont.)

	Near Term	Mid Term	Long Term
#9 Estimation & Reduction of Uncertainty			
We have identified and understand the sources of uncertainty for monitoring and modeling vadose zone sites.	◆		
We have assessed and catalogued the state-of-the-art methods for estimating and reducing uncertainty.	◆		
We have developed and tested new probabilistic approaches for estimating and reducing uncertainty.		◆	
We can optimize characterization and monitoring systems to reduce uncertainty, and we can predict the value of additional data for reducing uncertainty.		◆	
Site assessment models incorporate techniques for estimating and reducing uncertainty in making decisions on site cleanup and stewardship.			◆
#10 Improving Monitoring Systems			
Several conceptual models for fate and transport (beginning a catalogue) have been validated with field data representing an emerging set of standard monitoring approaches.	◆		
Researchers, site operators, regulators and stakeholders can access a catalogue of proven fate and transport models with data sets for priority vadose zone cleanup sites.	◆		
Real-time monitoring systems at sites with vadose zone contamination provide early warning of contaminant discharge or movement.		◆	
The model catalogue has been condensed and updated, and monitoring approaches have been standardized.			◆
#11 Integrating and Validating Site-Wide Models			
We can compare modeling techniques using a standard set of synthetic test problems.	◆		
We have models for sampling events and instrument response to improve instrumentation and network design for characterization and modeling.	◆		
We can test and validate models and measurement methods in laboratory and field experiments following standard protocols.		◆	
Site-wide assessment models are credible to both scientific and public policy communities.			◆
#12 GHCB Data Library and Model Set			
A virtual library of qualified GHCB data for priority contaminated sites is available to researchers, site operators, regulators, and the policy communities.	◆		
Virtual library data can be run on prototype models that incorporate a GHCB framework.		◆	
We can simulate critical features of priority contaminated vadose zone sites using GHCB models and virtual library data.			◆
#13 Sensors, Instrumentation & Emplacement			
Prototypes of miniaturized sensors are small enough to fit a package of 10 inside a two-inch hole.	◆		
We can characterize the geology and hydrology of a site at a 10-meter scale with one month turn-around.	◆		
Techniques to minimize emplacement effects have been developed and tested.	◆		
Minimally invasive emplacement methods and miniature sensors are available as alternatives to conventional boreholes and instrumentation techniques.		◆	
We can characterize the geology and hydrology of a site at 1-meter scale with a one day turn-around.		◆	
Injectable, smart sensors are available off the shelf; non-invasive methods for measuring key flow and transport properties are available.			◆
We can characterize the geology and hydrology of a site at 1-meter scale in real-time for most sites.			◆

Table 20 Highlights of Expected Results from Roadmap Activities (cont.)

	Near Term	Mid Term	Long Term
#14 Design & Optimization of Measurement Networks			
We can access a numerical laboratory linked with instrumented field sites to conduct experiments on characterization/monitoring network design and data value.	◆		
We can use field data in a numerical laboratory to optimize monitoring networks for field-scale experiments.		◆	
We can use network optimization design methods to explain cost-benefit risks and other trade-offs to end users, as part of planning for long-term monitoring and site assessment activities.			◆
We can quickly determine the location sensitivity and data value for designs of monitoring and characterization networks.			◆
#15 Facilities for Integrated Field Experiments			
Facilities to support IFEs have been constructed at representative sites.	◆		
Results from the first series of short-term IFEs are available.		◆	
Results from major, long-term IFEs are supporting and testing long-term research efforts, improving monitoring systems, and validating integrated assessment models.			◆
#16 The Problem Solving Environment			
We can access a shared PSE (software), which includes a common data structure for use in characterization, monitoring, and modeling, as well as a limited set of numerical modeling tools.	◆		
An extended PSE, linked to a geographical information system, incorporates a range of numerical methods and provides a computational test bed for validating models.		◆	
The vadose zone PSE incorporates realistic models for all coupled GHCB phenomena and state-of-the-art numerics; it supports 'value of information' assessment for monitoring and characterization systems.			◆
#17 Advanced Numerical Algorithms			
Existing state-of-the-art numerical methods have been adapted to address vadose zone problems.	◆		
A wide range of numerical methods relevant to vadose zone problems are available.		◆	
Site assessment models can automatically select the best numerical method at a spatial and temporal scale to minimize numerical error in decision variables.			◆
#18 High-Powered Computing			
A proposal is submitted to DOE and acquisition of the EHPCC begins.	◆		
First generation EHPCC is in use.		◆	
Second generation EHPCC is in use.			◆

5.1.1 Near-Term Outcomes: Moving Knowledge into Practice

Many of the near-term results in Table 20 share a common theme: *moving the state of the art to the state of practice*. This means getting the current knowledge and capabilities already existing in the research communities into operational use—for example, in developing monitoring strategies—at the nation's priority sites of vadose zone contamination. Some of the near-term results highlighted in Table 20 make this point explicitly, such as near-term results for Physical Description of Flow and Transport, the GHCB virtual library, or Estimating and Reducing Uncertainty:

- *Computer models used by federal agencies and others incorporate the best state-of-the-art conceptual models and implementations (software models).* (For details, see Activity PH5 in Section 2.2.1.)
- *A virtual library of qualified GHCB data for priority contaminated sites is available to researchers, site operators, regulators, and the policy communities.* (See Activity G1 in Section 4.1.1.)
- *We have assessed and catalogued the state-of-the-art methods for estimating and reducing uncertainty.* (See Activities UC1 and UC2 in Section 3.3 for details.)

In addition, many other near-term results contribute implicitly to this major outcome. For example, the near-term results for Chemical Properties and Processes include extending existing models for reactions in solution to the higher temperatures and ionic strengths often found in vadose zone environments (see Activity CH1 in Section 2.3.1.1). The near-term task for the model integration and validation Activity IV2 (Section 3.5) is to define synthetic test problems for comparing existing techniques of inverse modeling and model validation. In the activities to develop infrastructure and capabilities, the first near-term status point for Activity SIE1 is to demonstrate known techniques for sensor emplacement that could minimize effects on the vadose zone system, such as microdrilling and the use of coiled tubing (Section 4.1.2).

Moving state-of-the-art techniques and understanding into practice quickly has at least two significant benefits, one obvious and another less so. The obvious benefit is that these tasks "pick the low-hanging fruit," providing quick returns because much of the research investment has already been made. The less obvious benefit is that concerted effort to get new knowledge and technical capability into practice will bring researchers and solution-oriented problem owners into continuing and close interaction.

5.1.2 Mid-Term Outcomes: Improvements in Site Monitoring

For the mid-term, the roadmap outcomes of greatest significance are likely to be the cumulative *advances in monitoring systems* for vadose zone sites. The mid-term results in Table 20 that represent these advances explicitly include those for Improving Monitoring Systems; Sensors, Instrumentation, and Emplacement; and Design and Optimization of Measurement Networks:

- *Real-time monitoring systems at sites with vadose zone contamination provide early warning of contaminant discharge or movement.* (See Activities MON1 and MON3 in Section 3.4.2.)
- *Minimally invasive emplacement methods and miniature sensors are available as alternatives to conventional boreholes and instrumentation techniques. We can characterize the geology and hydrology of a site at 1-meter scale with a one day turn-around.* (See Section 4.1.2)
- *We can use field data in a numerical laboratory to optimize monitoring networks for field-scale experiments.* (See Section 4.1.3.)

Many near-term results and other mid-term results will contribute implicitly to advances in vadose zone monitoring capabilities. Improvements in both process understanding (quantified and tested through process modeling) and measurement capabilities will contribute to better monitoring systems. For example, the near-term and mid-term results highlighted in Table 20 for Biological Processes and Properties will improve monitoring of natural attenuation and in situ engineered bioremediation. The near-term and mid-term results for Multiphase Flow and Transport and Unstable Processes will aid in designing effective vadose zone monitoring systems and interpreting the data collected from them. Advances in scaling and early results from integrated field experiments are other examples of important contributions to improved monitoring capabilities.

A sound and efficient monitoring program is critical at major sites during environmental cleanup and afterward, throughout any period of stewardship required by residual contamination on site. The state of practice, enshrined in federal and most state environmental regulations, has been to monitor the groundwater at and around the site, rather than monitoring the vadose zone.[15] Where contaminants lie very close to the annual high water table, or for contaminants that move rapidly through whatever vadose zone separates the source term from groundwater, there may be no alternative. However, for many sites of serious subsurface contamination across the nation, waiting until contaminants appear in the groundwater means that a major part of the battle has been lost. If remediation can remove or isolate source terms and halt plumes while they are still in the vadose zone, the effectiveness of the remediation is often greatly enhanced, and the cost significantly reduced, compared with groundwater remediation alternatives. (See accompanying box on Dynamic Underground Stripping versus pumping and treating groundwater.)

5.1.3 Long-Term Outcomes: Accepted, Credible Support for Decisions on Environmental Cleanup and Stewardship

Many of the long-term results highlighted in Table 20 provide *better tools for supporting site-wide assessments and decisions* on environmental cleanup and stewardship. In truth, the Committee expects models and data gathering to improve year

[15] The state of federal regulation and regulatory practice with respect to vadose zone monitoring is discussed by Lorne Everett in the First Foreword in *Vadose Zone Science and Technology Solutions* (Looney and Falta, 2000, p. xix)

Stopping Contaminants in the Vadose Zone Versus Groundwater Remediation

Beginning in the 1980s, DOE-sponsored research at Lawrence Livermore National Laboratory (LLNL) developed and patented processes for removing or pyrolyzing subsurface petroleum and chlorinated hydrocarbons. This technology, called Dynamic Underground Stripping (DUS) and Hydrous Pyrolysis Oxidation (HPO), uses a control technology, cross-borehole electrical resistance tomography, to monitor the progress of the extraction and manage the steam front in the subsurface. DUS/HPO was demonstrated in 1994 on a deep gasoline spill at LLNL. In 1997 it was implemented as an alternative to conventional pump-and-treat of groundwater at a utility pole creosoting yard in Visalia, California (the Visalia Pole Yard). The table below compares this vadose zone remediation alternative with pumping and treating groundwater. In addition, pump-and-treat remediates only the groundwater, whereas DUS/HPO remediates contamination in both the vadose zone and the groundwater.

Project Parameter	LLNL Gasoline Spill	Visalia Pole Yard
Total project cost ($ millions, through 2000)	$11	$21
Unit cost per cubic yard of soil treated		
Actual cost	$65	$57
Predicted repeat cost (w/ lessons learned)	NA	$38
Costs without research component	$35	NA
Comparative cost per gallon of creosote removed		
Pump and treat groundwater	NA	$26,000
DUS/HPO vadose zone remediation	NA	$130
Time to remove 7,600 gallons of gasoline (LLNL) or 1.3 million pounds of creosote (Visalia)		
Pump and treat groundwater	**2,000 years**	**3,250 years**
DUS/HPO vadose zone remediation	**1 year (estim.)[a]**	**3 years**

NA = data not available or not applicable
[a] The LLNL demonstration operated for only 15 weeks. The estimate is based on yields obtained during the demonstration.
Source: Everett, 2001.

by year even in the near and mid-term. However, after a decade or so of pursuing the roadmap's activities, the Committee anticipates a qualitative leap forward. We will then be able to visualize, quickly and accurately, the current state of site-wide (and larger) vadose zone systems. We will be able to simulate their behavior under multiple alternative future scenarios, reaching to the long time horizons required to support major cleanup and stewardship decisions. These projections, which will carry levels of certainty and sensitivity unattainable at present, should suffice to win the confidence of regulators and the public.

Results from many parts of the roadmap will contribute to this major pay-off. The ultimate goal is captured in the long-term result for Integrating and Validating Site-Wide Models:

- *Site-wide assessment models are credible to both scientific and public policy communities.*

Among the technical capabilities that site-wide assessment models will have to incorporate to attain this credibility are those noted in the long-term status points, as well as mid-term tasks and status points. Additional relevant capabilities are expressed in the long-term results highlighted in Table 20 for categories 1 through 9, 12, and 15 through 18. Even a glance through these for Activities IV1 through IV4 (Section 3.5), the highlighted summary results, show that a great deal of work must be undertaken and completed successfully to reach the ultimate goal.

5.2 Linkages Among Research and Infrastructure Activities

The activity structure used in Sections 2 through 4 establishes connections among the tasks and status points under an activity. However, the connections across the activities, particularly those between research areas and infrastructure development, are only partially represented, for instance by cross-cutting status points for the most important linkages. A great many more interdependencies among these efforts can be identified, even at this planning phase. More will arise unexpectedly as work is done, provided there is ample communication across disciplines and specific applications.

Linkages that are important for roadmapping include *prerequisites, influencers,* and *synergies*. An effort ***x*** has a *prerequisite* ***y*** if ***x*** cannot occur (or is not expected to occur) unless ***y*** also occurs. An effort ***x*** *influences* ***y*** if progress in ***x*** affects progress in ***y***, but ***y*** could occur without ***x***. Two efforts are synergistic if progress in either is likely to occur more quickly, or advance further, if the other progresses. Prerequisites are important for S&T planning because they shape the critical path to important outcomes. Synergies and influences are important as opportunities for communication and cooperation that can produce desired outcomes more quickly and efficiently.

Many of the crosscutting status points for the roadmap activities represent developments that have prerequisites in the activities they connect. For example, the two cross-cutting long-term status points for Activities PH10 and PH11 (see end of Section 2.2.3) will not occur unless there is progress in both defining the relationships by which geophysical attributes can be translated into flow and transport parameters (Activity 10) and applying improved geophysical measurement technologies at typical sites of vadose zone contamination (Activity 11).

In other instances, the cross-cutting status points reflect synergies rather than strict prerequisites. The two cross-cutting long-term status points for coupling basic properties and processes (Section 3.1) are more likely to be achieved with success in all three of the CP activities (better databases for processes with GHCB properties, cross-disciplinary modeling approaches, and realistic models for strongly coupled nonlinear phenomena). In addition, progress in Activity CP3 (realistic models for strongly coupled nonlinear phenomena) is almost certainly a prerequisite for both of these status points.

As the Executive Committee worked on refining the structure of this initial roadmap, a particularly critical set of linkages emerged between the research activities in Sections 2 and 3 and the infrastructure activities in Section 4. As noted in the introduction to Section 4, early progress on a number of the infrastructure activities depends on near-term research efforts to move the state of the art into practice. If these dependencies are not strict prerequisites, they are at least very strong influences on the rate and extent of infrastructure development for a given level of resource investment. Examples include assembling the GHCB virtual library, developing the first release of the vadose zone

PSE, and setting up the site instrumentation, numerical laboratory support, and other facilities for one or more IFE sites.

Once these infrastructure capabilities are operational, even as "first generation" implementations, they will exert strong accelerating influences on the mid-term and long-term progress in most of the research activities in Sections 2 and 3, including those on which they initially depended. Looking at the research activities and the infrastructure development activities as program elements, there are strong synergies between them. The opportunity this represents argues for programming investments in both areas with an eye to achieving the greatest boost from their synergies.

A wall chart of the highlighted results in Table 20, which captures important linkages at the level of major results for the three time horizons, is available from INEEL. In subsequent refinements and updates of this roadmap, it would be useful to trace and document these dependencies, particularly the prerequisites and strong synergies for key outcomes, at a more detailed level. Specific tasks or status points that have prerequisites or strong synergies need to be identified. The key outcomes should be those that participants agree are most important to the goal of protecting groundwater resources from vadose zone contamination.

5.3 Vadose Zone Research in the Context of Environmental Cleanup and Stewardship Imperatives

This roadmap covers only a part of the effort needed for environmental cleanup and stewardship of the nation's vadose zone contamination problems. It does not cover the S&T for remediation and isolation techniques or other modes of action for exercising stewardship in the broadest sense. Nor does it include the S&T to support assessment of impacts on human health, the environment, and the local, regional, or national economy.[16] Beyond even the S&T components, there are many other factors in the conduct of cleanup and stewardship operations. Regulatory requirements, the concerns and interests of affected communities and other stakeholders, legacy contracts and operations, and competing uses of scarce resources are among the factors that form this broader context.

An analysis of linkages in terms of prerequisites, influences, and synergies can be applied here, as well as to the roadmap activities. Results of activities outlined in this roadmap will affect the S&T activities for contaminant removal, immobilization, or other cleanup operations, as well as choices among active cleanup and natural or engineered attenuation. Progress in the S&T for those activities will in turn influence the work needed in site visualization and monitoring systems, sensor and measurement techniques, and even the required degree of understanding of various vadose zone processes. More broadly, achieving near-term results such as those highlighted in Table 20 will influence

[16] Although these other aspects of the total environmental cleanup and stewardship effort are not specifically included in this roadmap, moving predictive tools described here from the state of the art to state of practice and implementing the infrastructure and capabilities will support these wider activities.

the support from stakeholders and government budgeting authorities for further efforts to understand, monitor, and control contaminants in the vadose zone. In this light, it is important for the roadmap presented here to be integrated with the larger context of S&T planning for cleanup and stewardship. Efforts in planning for the larger context will require refining and updating this roadmap.

One significant element of the larger context that affects this roadmap is the sense of urgency, conveyed in regulations as well as in political and social drivers, to clean up environmental contamination quickly before more damage is done. In meetings with regulators, other stakeholders, and site cleanup operators, a plan like this for "more research," particularly for long-term research, often raises concerns that doing more research will divert resources and attention from cleanup. If cleanup plans are already formulated, agreed upon, and prescribed by regulatory authorities, why is long-term research needed? For DOE's cleanup sites, this issue is sharpened by site-specific timetables, often formalized as regulatory requirements, to "clean up and close" DOE operations on most or all of a site by a specified date. "Closure" in this sense implies an end (or major downsizing) to expensive tax-supported operations and a return of all or most of the site to other uses.

Whenever the resources needed for a range of potential activities are limited, there is potential for competition among those activities. In that sense, any activity in this roadmap may "compete" for resources with another roadmap activity. And a program to pursue the roadmap systematically can be viewed as competing with any other national program, from defense to health care to debt reduction, as well as programs for environmental remediation. However, to focus on just the potential for resource competition is to ignore the considerable potential for constructive influences and synergies, which a systematic approach to resource allocation can tap. *A well-planned program for research and development to improve cleanup and stewardship options can, and should, be a profitable return on investment for the nation.* The reason for performing this roadmapping activity was to improve and extend just such a planning process, continuing forward from preceding and concurrent efforts at DOE and elsewhere.

Recent research on alternative landfill covers to meet requirements of the Resource Recovery and Conservation Act (RCRA) illustrates the investment potential of research. (See accompanying text box.) This example also points out some of the fallacies in a simplistic view of "finishing" cleanup operations. At many national priority sites, the planned cleanup operations will leave residual wastes in the subsurface, often in the form of waste burial grounds, landfills, or other relatively concentrated "waste inventories." In many instances, a land cover similar to those tested in this research will be used to minimize the flow of contaminant-transporting water through the zone of buried waste.

In the land cover study, the installation cost of the successful alternative (the evapotranspiration cover) was half that of the prescribed approach with equivalent performance (the RCRA Subtitle C cover). A simpler and less expensive prescribed approach (approved for sanitary landfills) failed in the climatic and soil conditions of the test. More important, though, the estimated operating and maintenance cost for the

Alternative Land Cover Research as a Stewardship Investment

Sandia National Laboratories tested the performance of six alternative approaches to an engineered landfill cover in an arid to semi-arid environment typical of the western U.S. The five-year project was funded by the EPA, the DOE Subsurface Contaminants Focus Area, and the DOE Characterization, Monitoring and Sensors Technology Crosscut Program. Two of the designs were those prescribed in RCRA Subtitle C (RCRA C cover) and RCRA Subtitle D (RCRA D cover). Of the four experimental designs tests, the anisotropic barrier cover and the evapotranspiration soil cover had flux rates and barrier efficiencies similar to that of the RCRA C cover. The anisotropic barrier incorporates soil layers that facilitate the lateral movement of water through drainage layers within the barrier. The evapotranspiration cover uses soil mixtures and compaction to hold moisture near the surface, where a mix of surface vegetation recycles nearly all of it to the atmosphere by evaporation and transpiration. Based on the results summarized below, the evapotranspiration design was selected for installation over a mixed waste landfill at Sandia National Laboratories.

Cover Design	RCRA D	RCRA C	anisotropic	evapotranspiration
Flux rate (mm/year)	4.82	0.13	0.16	0.19
Barrier efficiency	99.986%	99.999%	99.999%	99.999%
Construction cost ($/m^2)	$51.40	$157.54	$75.26	$73.89
Landfill Application ($million)				
Total capital cost	not reported	$3.55	not reported	1.76
Operation & maint., 30 yr.	not reported	$12.36	not reported	$2.07

Source: DOE, 2000

alternative for 30 years "after closure" is one-sixth of the equivalent cost for the RCRA Subtitle C cover. The primary cost for operation and maintenance is for long-term monitoring to ensure the cover does not fail. Whereas the prescribed approaches require groundwater monitoring wells and laboratory analysis of collected samples, the alternative employs embedded fiber-optic moisture sensors that do not require laboratory analysis.

The alternative barrier designs in this research all are based on principles for limiting percolation of infiltrating moisture through the layers of soil or sand. They thus depend on understanding vadose zone flow and transport processes. The alternative monitoring approach reflects advances in measurement methods, including sensor instrumentation, applicable to monitoring in the vadose zone. If the cost savings for the alternative , compared with the RCRA Subtitle C cover, are multiplied by just the number of DOE and other hazardous waste landfills in similar environments, the "return on investment" for this research is huge. These savings do not even reflect avoiding the additional costs of cleaning up or isolating contaminated groundwater if RCRA Subtitle D covers were to be used on sanitary landfills in environments where they quickly fail.

5.4 Interagency and Intergovernmental Coordination is Critical

This roadmapping project began with an emphasis on vadose zone S&T needs for cleanup and stewardship at the DOE sites, particularly those where vadose zone contamination would remain a stewardship issue for decades. The initial objective was to create a DOE complex-wide roadmap first, and then consider the extent of its applicability to other situations, including vadose zone contamination issues being addressed by other federal agencies (e.g., Department of Agriculture, DOD, EPA, and the U.S. Geological Survey). However, as the details of needed research were compiled by the three work groups listed in Appendix A, the Executive Committee and DOE sponsors realized that even this initial set of activities would have broad applicability beyond DOE's cleanup needs. This draft (Revision 0.0) has been extensively revised to express this broader relevance, even though the participation by other agencies to this point has been limited.

Given the broad potential applicability of the S&T work identified here—and the sheer scale of the effort that implementation will require—a coordinated approach involving all of the agencies named above, and perhaps others,[17] is essential. From this perspective, the current version of the roadmap is unquestionably a first step for consideration and revision in some subsequent context where the other agencies are more fully involved as partners with the DOE. Precedents such as the interagency coordination on the U.S. Global Climate Research Program provide the Executive Committee with hope that its attempt to reach beyond DOE sites will not fall on deaf ears.

This cooperation in further shaping a national roadmap for vadose zone S&T should extend even beyond the federal sphere. States and local governments face significant problems related to vadose zone contaminant transport. The contaminants typically derive from industrial sites, suburban septic tanks, old gasoline stations and petroleum distribution centers, agricultural activities, and municipal refuse rather than nuclear fuels production. Yet, much of the research results and infrastructure proposed here could help with their problems as well.

In addition, State health and environmental authorities are playing an increasingly active role in cleanup agreements with federal facilities. The communities near those facilities—or anywhere downgradient or downstream from them—are the people most directly impacted by the possibility or reality of groundwater contamination. Thus many linkages—prerequisites, influences, and synergies again—exist to tie the activities of DOE, DOD, and EPA with State and local governments. If this initial roadmapping exercise is sustained in some form, the Executive Committee believes there should be some mechanism to represent these broader constituencies in the process.

5.5 The Ultimate Driver: Protecting the Nation's Groundwater Resource

Despite the arguments stated above for the investment value of research or the necessity for cooperation across institutional boundaries, the Executive Committee knows that serious challenges and obstacles will confront any attempt to pursue and improve this ambitious roadmap. If the effort has not been futile, if in time a goodly share of the

[17] The vadose zone as a moisture and heat source and sink in models of atmospheric-terrestrial-oceanic coupling is emerging as an issue for refining projections of climate change due to accumulation of greenhouse gases. In this respect, the National Aeronautics and Space Administration (NASA) could be another entity to which this roadmap has relevance.

results are realized because sufficient support has been mustered and directed well, it will happen for one reason: the nation needs to protect its groundwater.

Throughout history, the fate of nations, and even of civilizations, has risen and fallen with the adequacy of safe water supplies: water for man and beast to drink, water to grow crops, sustain fertile soils, and form aquatic ecosystems. Increasingly we depend on the groundwater to meet our needs for potable water and irrigation. Even where we can tap surface waters for these purposes, the purity of groundwater that invisibly flows into surface drainages can become an issue. The United States has been blessed with abundant groundwater; its benefits are everywhere around us.

Unfortunately, we have only recently realized that transport of contaminants through the vadose zone can threaten the groundwater resource in ways our predecessors never considered. Once contaminants are in the subsurface, it is far better to stop them in the vadose zone than prevent their spread after they reach groundwater. The ultimate driver for significant investment of national treasure in the research and infrastructure activities contained in this roadmap is to protect an even more valuable national treasure, our groundwater resource.

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ACRONYM LIST

ASCI	Accelerated Strategic Computing Initiative
DOD	U.S. Department of Defense
DOE	U.S. Department of Energy
DUS	Dynamic Underground Stripping
EPA	U.S. Environmental Protection Agency
GHCB	Geological, hydrologic, chemical, and biological
GIS	Geographical information system
HPO	Hydrous Pyrolysis Oxidation
IFE	Integrated field experiment
INEEL	Idaho National Engineering and Environmental Laboratory
LLNL	Lawrence Livermore National Laboratory
MCL	Maximum Concentration Limit
NAPL	Non-aqueous phase liquid
NAWQA	National Water-Quality Assessment
PSE	[Vadose zone] problem solving environment
R&D	Research and development
RCRA	Resource Conservation and Recovery Act
S&T	Science and technology

APPENDIX A. ROADMAP CONTRIBUTORS

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APPENDIX B. TABLE OF ROADMAP ACTIVITIES WITH TASKS AND STATUS POINTS

#1 Physical Description of Flow & Transport

	Near Term	Mid Term	Long Term
Activity PH1: Assess the importance of fluid flow and chemical transport processes and subsurface properties relevant to site characterization, remediation and long-term stewardship.			
Status: Subsurface properties (e.g., gravitational, pressure, temperature and chemical gradients) of importance to fluid flow and chemical transport at contaminated vadose zone sites have been identified and assessed.			
Activity PH2: Design and conduct laboratory and field experiments to resolve critical gaps in understanding fluid flow and chemical transport processes in granular media. Criticality of gaps is to be assessed by relevance to environmental restoration and long-term stewardship missions of the DOE and other agencies.			
Status: Critical gaps that can be answered within a decade through lab and controlled field experiments have been identified and prioritized.			
Task: Design, implement, and analyze results of laboratory and field experiments for the prioritized critical gaps.			
Activity PH3: Improve process-based understanding and models for flow and transport in macroporous soils and unsaturated fractured rocks.			
Task: Develop realistic representations of pore-space geometry of, and fluid flow in, fractured media using geological, pedologic, and topological characterization techniques.			
Task: Develop and implement improved descriptions of matrix-fracture interactions.			
Task: Develop general constitutive relationships for both granular and structured media.			
Task: Develop pore network and other models based upon appropriate equations (e.g. Navier-Stokes), and devise methods for upscaling processes and/or properties from sample to formation scales.			
Task: Incorporate solid surface heterogeneity (pore and sample scale) with detailed hydrodynamics into solute transport models (to model opportunity times for reactions, streaming potentials, and other processes or variables).			
Activity PH4: Develop methods for modeling scale-dependent properties and processes and for assimilating data from different scales into these models.			
Task: Develop and implement improved models for evapotranspiration and root water uptake as a function of water stress and other factors.			
Task: Develop process-hierarchical approaches for describing and modeling controlling processes (e.g., models of increased complexity for flow in structured media, or increasingly sophisticated process-based approximations for gaseous transport or the flow of non-aqueous phase liquids).			
Status: Methods have been developed to quantify spatial variability in flow and transport parameters, fluid properties, thermal properties, and biological and chemical reactions			

#1 Physical Description of Flow & Transport (cont.)

	Near Term	Mid Term	Long Term
Task: Investigate potential of collecting/inverting multi-scaled data to provide information about variability as a function of scale.			
Task: To understand how different measurement methods scale from one level of support to another, experiment with modifying the acquisition parameters for a certain type of method to sample different scales of variability.			
Status: Methods have been developed for measuring physical processes and properties and their uncertainties across different scales. The multi-scale data from these methods can be assimilated into process models in which the properties and processes can be propagated (in simulations) as, for example, governing equations, driving forces, and/or media properties.			
Status: Linkages between relevant small-scale processes and properties with larger-scale flow and transport behavior have been identified for cases where no simple upscaling is possible.			
Status: Microbiology modules are incorporated into physical models of solid-gas-liquid environments.			
Status: Solid surface evolution due to biogeochemical reactions (precipitation-dissolution, reduction-oxidation, and other reactions that can change solid-phase geometry and density of exchange sites) has been incorporated into transport models necessary for long time-scale simulations.			
Status: Models for unsaturated flow and transport in different types of porous media have been developed that are both process-adaptive and scale-adaptive. These models invoke the appropriate processes at the appropriate scale and employ the corresponding transport and hydraulic properties.			
Activity PH5: Improve the state of practice in flow and transport models used by government agencies for VZ contamination simulations, beginning with DOE.			
Status: DOE flow and transport prediction models and solutions have been updated by incorporating known models/modules with a more sound physical-chemical basis.			
Task: Integrate critical elements of chemistry and microbial activity in models for liquid flow and solute transport.			
Activity PH6: Develop, improve, and confirm of methods for measuring basic hydrologic properties.			
Status: Moisture content, matric potential, and temperature measurements are no longer a major source of uncertainty for site-wide monitoring and modeling. Monitoring approaches for these properties are robust enough to cover long-term stewardship responsibilities.			
Activity PH7: Improve the capability to track subsurface fluid flows with increased precision, over larger areas, and at greater depths underground.			
Status: Improved resolution and decreased uncertainty. Example, fluid movement (such as in an infiltration event) in a 10 m X 10 m area, at depths up to 100 m, can be tracked to a precision of 10 percent.			

#1 Physical Description of Flow & Transport (cont.)

	Near Term	Mid Term	Long Term
Status: Further improvements in resolution and uncertainty reduction. Example: fluid movement in a 50 m X 50 m area, at depths up to 100 m, can be tracked to a precision of 5 percent.			
Status: Greatly improved resolution and reduced uncertainty. Example: a three-dimensional pulse of water (2 m X 2 m) can be identified to a precision of 2 percent at depths up to 100 m.			
Activity PH8: Optimize the use of natural and anthropogenic tracers for determining directions and rates of transport, assessing flow processes, and validating numerical models.			
Task: Develop, test, and confirm the inverse process of using tracers to estimate fluxes and ages of pore water. Include methods to propagate uncertainties in tracer measurements to obtain uncertainties in calculated fluxes and ages.			
Status: A variety of tracers are available for use in locating contaminants, establishing the role of surface boundary conditions in specific subsurface environments, and obtaining point estimates of fluxes and ages.			
Activity PH9: Develop capability to detect the presence and movement of fluid in fractures and fracture networks.			
Status: The presence of fluid in individual fractures can be detected in some cases.			
Task: Quantify the relationships among the most likely geophysical methods or combinations of methods that will provide fracture diagnostics.			
Status: Contaminant fluid in fractures can be detected in most cases.			
Task: Discover and quantify new relationships between surface geophysical measurements and fractures, so that fractures a few centimeters across at depths of 10 meters can be routinely mapped.			
Status: Contaminant fluid in fractures in real time can be detected and quantified from the surface or in boreholes.			
Status: Low-cost, automated, and reliable geophysical techniques are available for mapping fractures immediately at the field site, without delays for processing or analysis.			
Activity PH10: Characterize the petrophysical relationships for translating geophysical attributes in near-surface strata into estimates of hydrologic parameters relevant to vadose zone contamination (e.g., porosity and water content).			
Status: Generalized petrophysical relationships between geophysical attributes and hydrologic parameters have been developed for near-surface environments.			
Task: Investigate how multiple types of geophysical and other data reduce uncertainty in applying petrophysical relationships and can aid in resolving issues of non-uniqueness in relationships between geophysical and hydrologic parameters.			
Status: The mechanisms of geophysical energy propagation at the field tomographic scale within unconsolidated or loosely consolidated, low pressure, granular porous material are understood.			

#1 Physical Description of Flow & Transport (cont.)

Near Term | Mid Term | Long Term

Status: Joint and constrained inversions that honor all data can be performed. How additional data improve the estimate and decrease the estimation error is understood. Data with different measurement scales can be incorporated in the inversion process correctly.

Task: Develop a quick and reliable way to assess the scale of a vadose zone contamination problem relative to the scale of the hydrologic heterogeneity so that the most appropriate techniques and acquisition parameters can be selected for characterizing the key parameters that control flow and transport at that site.

Status: Methods to scale between lab-scale and field-scale measurements are known and in use. A variety of differently scaled data can be reliably incorporated into geophysical inversions to provide an integrated and hierarchical interpretation of hydrologic properties.

Activity PH11: Improve and apply geophysical methods for characterizing near-surface environments typical of sites with vadose zone contamination.

Task: Develop automatic data picking and quality control approaches for crosshole tomographic methods.

Task: Investigate the utility of constrained and joint inversion for improved estimation of hydrologic parameters. Develop stochastic inversion procedures that yield distributions of possible geophysical attributes at each location.

Status: Stochastic estimation techniques that provide an estimate of the property of interest, as well as information about its uncertainty, have been tested and applied to contaminated vadose zone sites.

Status: Incorporate measurement support scale, and other means of recognizing the importance of scale, when applying geophysical methods to estimate hydrologic properties and correlation lengths.

Status: Hydrologic properties (e.g. water content, permeability and porosity) and their associated uncertainties and spatial correlation functions are being estimated from different types of geophysical data such as crosshole tomographic imagery. These estimates are conditioned to direct measurements, with attention to scale, using hierarchical spatial scale estimation procedures with multi-scaled data.

Activities PH10 and PH11:

Status: Practical guidelines for different environments allow quick field tests to determine the characterization regime into which the vadose zone at a contaminated site falls. The governing petrophysical relationship for that regime is used to interpret the geophysical data to obtain first-pass estimates of key flow and transport parameters.

Status: Tomographic methods can supply real-time, multidimensional (spatial and temporal), automatic interpretations of hydrologic properties or changes in properties due to bacterial modification, environmental remediation, infiltration, and other dynamic processes. The fully automated inversion process may also incorporate varying scales, but must provide real-time estimates of hydrologic properties at high resolution.

HIGHLIGHTS OF EXPECTED RESULTS

Computer models used by federal agencies and others incorporate the best state-of-the-art conceptual models and implementations (software modules).

We can detect the presence of fluid in fractures in some cases.

We can distinguish, in most cases, the subset of fractures that are conduits for fluid flow and contaminant transport.

We can map and predict water distribution and flow through structured soils or fractured rock at multiple spatial scales.

Monitoring data on fluid flow and contaminant transport can be interpreted and represented visually at site-wide scales in real-time.

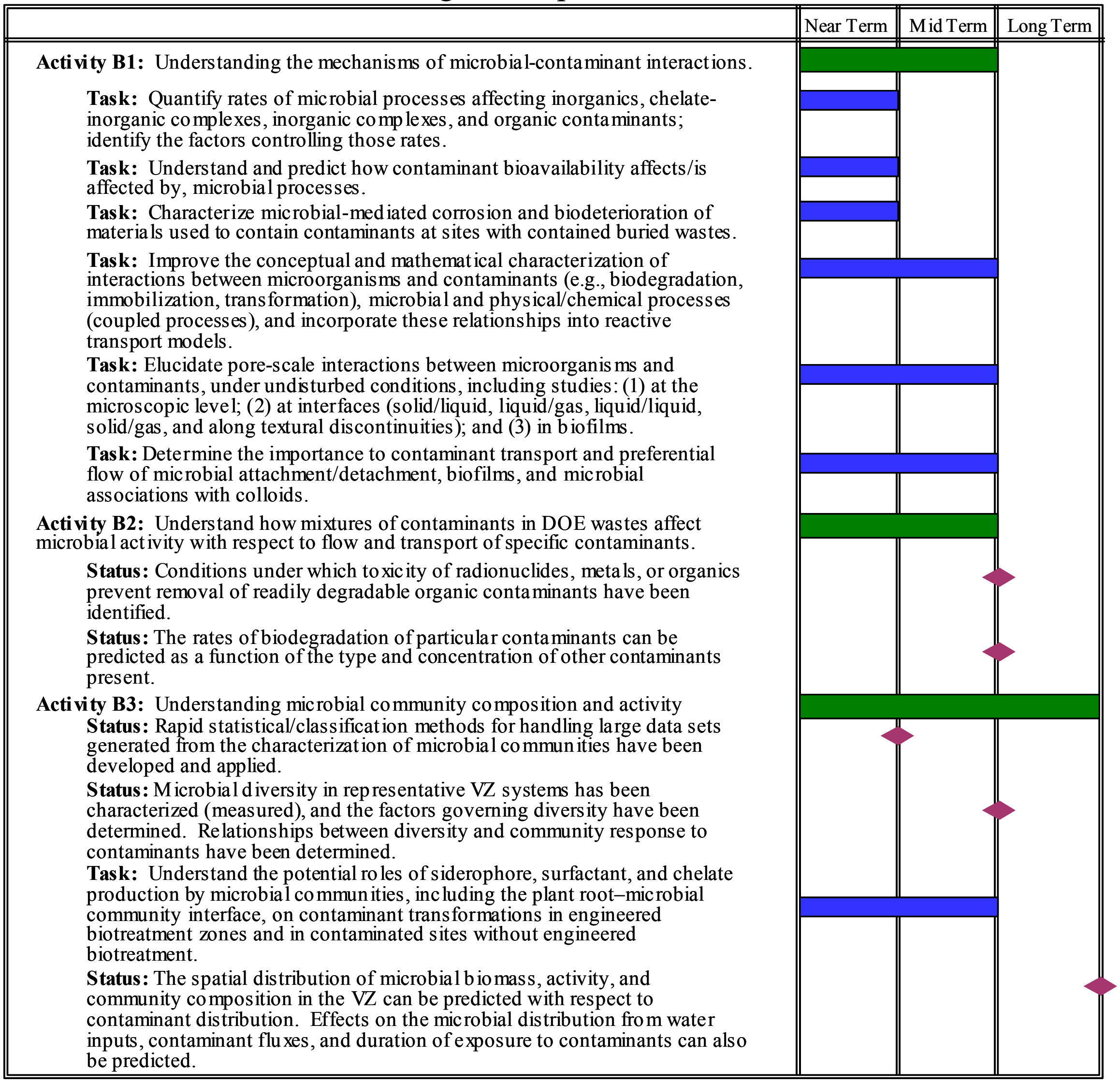
#2 Chemical Properties & Processes

	Near Term	Mid Term	Long Term
Activity CH1: Extend solution chemistry models to higher temperatures and ionic strengths (e.g., Pitzer equations) relevant to VZ contamination problems.			
Status: Solution chemistry models have been extended to temperatures and ionic strengths needed for most VZ contamination problems, including DOE contamination sites.			
Activity CH2: Improve the understanding of kinetic rate mechanisms and effective surface areas, in order to develop improved rate laws.			
Status: Reaction kinetics and rate laws have been formulated that are appropriate for use in numerical continuum models of reactive flow and transport for many VZ contamination problems, including DOE sites.			
Status: Databases of appropriate reaction rate constants applicable to refined reaction rate laws have been developed through experimental studies.			
Activity CH3: Investigate cation exchange capacity and surface site density/complexation reactions on mineral surfaces and colloids for systems typical of VZ environments and contamination problems. Resolve the importance of lack of charge conservation in surface complexation models when combined with transport, possibly by including streaming potentials in the formulation.			
Task: Determine if significant differences exist for measurement of cation exchange capacity and surface site density between *in situ* field measurements of undisturbed samples and lab batch measurements involving disturbed media. Validate conditions under which batch K_d measurements can be used to estimate retardation in variably saturated flowing systems.			
Status: The kinetics (including reversibility) of ion exchange and surface complexation reactions on mineral surfaces and colloids has been determined for most solution-solid systems relevant to VZ contamination problems.			
Activity CH4: Investigate the effects of dissolution and precipitation on porosity, pore structure, and permeability. Study nucleation controls that may bias dissolution and/or precipitation to particular pore environments.			
Task: Develop a functional description for porosity/permeability evolution reflecting chemical effects.			
Task: Develop rate laws for glass dissolution and solid solutions that cover more extended conditions typical of natural and contaminant-affected flow fields. Improve models of nucleation processes.			
Activities CH1 through CH4: **Status:** Kinetics and rate laws have been formulated for ion exchange and surface complexation processes coupled with mineral precipitation and dissolution. This knowledge has been validated in field experiments and incorporated in reactive flow and transport models for VZ systems.			

#2 Chemical Properties & Processes (cont.)

	Near Term	Mid Term	Long Term
Activity CH5: Investigate phase boundary conditions occurring in VZ environments that may significantly influence liquid flow and contaminant transport.			
Task: Develop accurate models for mineral reactions in contact with a thin liquid film that may have different properties compared to bulk fluid (e.g., for extreme evaporation conditions that may favor formation of evaporite mineral phases).			
Task: Develop accurate models for mineral reactions in unsaturated systems having variable gas phase chemistries (e.g., low and high CO_2 or O_2).			
Activity CH6: Improve and develop methods of identifying chemical contaminants in the VZ.			
Status: The presence of individual chemical contaminants in soils or other VZ strata can be determined from surface or borehole measurements, although field results may require verification with lab analyses.			
Status: Concentrations of the most abundant species (except those at very small concentrations) can be determined within an order of magnitude.			
Status: Contaminated volumes can be isolated, and the concentration of abundant chemical species can be determined to within 10 or 20 percent.			
Status: The volumes and spatial distributions of resident contaminants at or near source discharge points can be quantified for metals, radionuclides, and organics.			
HIGHLIGHTS OF EXPECTED RESULTS			
Reaction kinetics and rate laws (in solution) have been formulated for priority vadose zone conditions.			
Individual chemical contaminants in the vadose zone can be detected.			
We understand the kinetics for important chemical reactions at solid and liquid interfaces (e.g., ion exchange and colloids) in vadose zone conditions.			
Flow and transport models map and predict important vadose zone chemical interactions, including those involving mixtures of solids, liquids, and air.			

#3 Biological Properties & Processes



#3 Biological Properties & Processes (cont.)

	Near Term	Mid Term	Long Term

Activity B4: Characterization methods to understand *in situ* rates and community activities at scales relevant for field-scale modeling.

- **Task:** Characterize microbial transport in different natural porous media and through/from engineered biotreatment zones relevant for VZ contamination sites (DOE and others). In particular, characterize transport through unsaturated fine and coarse sands and fractured rock, as a function of water saturation and solution chemistry.
- **Status:** *In situ* rates of microbial biotransformation of contaminants at contaminated sites (DOE and other VZ sites) can be predicted as a function of site and environmental conditions.
- **Status:** Information about the composition of VZ microbial communities has been incorporated into pollutant fate and transport models.
- **Status:** Transport of native and introduced microorganisms at contaminated VZ sites (DOE and others) can be predicted.

Activity B5: Developing and improving measurement techniques for bioavailability.

- **Status:** Improved bioavailability sensors and/or assays have been developed.
- **Status:** *In situ* bioavailability sensors have been developed and are in application.

Activity B6: Developing and applying sensors and sensor systems for *in situ* rate measurements.

- **Status:** Sensors and systems for *in situ* rate measurements have been developed.
- **Status:** Chemically reactive contact foils and films for *in situ* rates and/or potential activity have been developed.

Activity B7: Developing and applying systems for measuring microbial community composition and activity.

- **Status:** Sample-to-answer analytical systems for community composition and activity have been developed.
- **Status:** Spectroscopy-based and synchrotron-based inferences of microbial activity have been developed.
- **Task:** Perform lab studies and develop models of the bio-electric level as a function of different soil types and microbes (aerobic versus anaerobic, a variety of metal-reducing and organics-reducing microbes).
- **Status:** Inexpensive sample-to-answer analytical systems for community composition and activity are being applied.
- **Task:** Develop instrumentation to detect lower levels of activity and validate this instrumentation in intermediate-scale and field-scale tests.

Activities B5 through B7:

- **Status:** Economical analysis of spatial distribution and temporal dynamics has been developed and applied.
- **Status:** Nondestructive joint measurement of biological, geochemical, physical, and hydrologic properties or processes has been extended to intact cores and possibly to the subsurface.
- **Status:** Proxy measurements for microbiological properties and processes have been developed.

HIGHLIGHTS OF EXPECTED RESULTS

We understand and can predict how microbial processes affect or are affected by bioavailability of important contaminants.

We can measure biochemical rates, in situ bioavailability, and the composition and activity of microbiological communities.

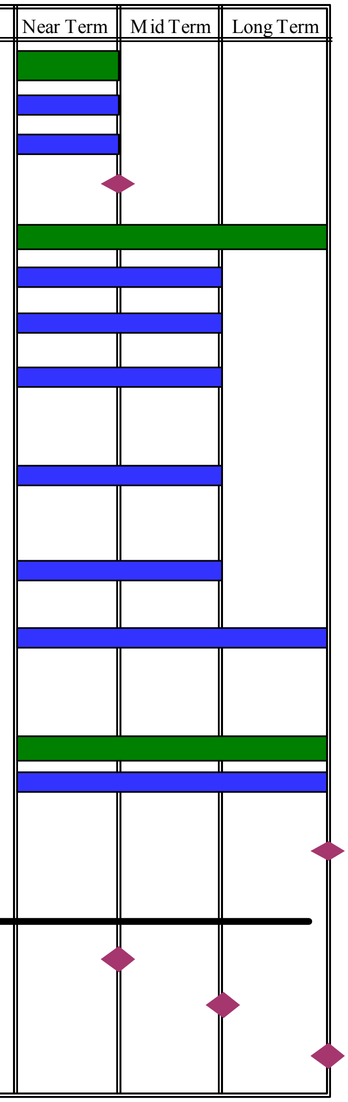
Reactive transport models can predict how microorganisms will interact with contaminants.

Inexpensive systems are available to measure community composition and activity.

We can accurately predict site-specific biodegradation rates for important contaminants.

We can take biological measurements along with others without destroying the samples.

#4 Colloidal Formation & Transport



Activity COL1: Improve sampling and analysis for colloids and colloidal transport.

- **Task:** Develop a scientifically based protocol for field based sampling and analysis for colloids and colloidally transported contaminants.
- **Task:** Develop new sampling techniques for *in situ* measurements of colloidal particles in pore water.
- **Status:** Mobile colloids are considered in sampling and analyses protocols for field studies and monitoring systems.

Activity COL2: Studies of colloidal transport.

- **Task:** Quantify effect of preferential flow on colloid transport.
- **Task:** Understand relevance of colloid-facilitated transport to contaminant movement under transient flow conditions, including wetting, drying, and infiltration processes.
- **Task:** Quantify the potential for *in situ* colloid formation and mobilization under conditions relevant for major VZ contamination sites, particularly in the presence of extreme chemical conditions that can lead to dissolution and precipitation of soil minerals.
- **Task:** Evaluate the effects on production and behavior of microbial colloids of (1) changing contaminant flux, (2) nutrient injection during engineered bioremediation, and (3) cell to cell communication (quorum sensing) in biofilms and other cell assemblages.
- **Task:** Characterize colloid-contaminant interactions as a function of solution chemistry and water saturation, at both microscopic and macroscopic levels.
- **Task:** Characterize colloid transport in different natural porous media relevant for sites with contaminated VZs, In particular, characterize and quantify colloidal transport through unsaturated fine and coarse sands and fractured rock, as a function of water saturation and solution chemistry. Quantify colloid interactions with solid-liquid and liquid-gas interfaces.

Activity COL3: Models of colloidal transport.

- **Task:** Model colloid transport and colloid-facilitated transport in unsaturated soils, sediments, and fractured rocks.
- **Status:** Improved conceptual and mathematical characterizations of colloid-contaminant-soil interactions and colloid-facilitated transport have been incorporated into reactive transport models used by DOE and other agencies for assessing VZ contamination.

HIGHLIGHTS OF EXPECTED RESULTS

We know how to detect mobile colloids and how to sample and analyze them.

Important colloid-contaminant interactions understood at micro and macro levels.

Flow and transport models can map and predict important colloidal interactions and transport.

#5 Multiphase Flow & Transport

Activity MP1: Extend knowledge and predictability of flow and transport processes to multiphase systems.

Task: Quantify effects of subsurface physical and biogeochemical heterogeneity on multiphase flow and transport processes.

Status: Upscaling procedures to apply lab-derived multiphase constitutive properties and parameters to the field scale have been developed.

Status: Process-based models can describe unstable and preferential flow of aqueous and NAPL phases.

Task: Conduct multiphase flow and NAPL transport experiments for representative soils and contaminants, to elucidate real-world problems and data limitations.

Activity MP2: Studies of key contaminant mixtures (for DOE and other contaminated VZ sites) as multiphase systems.

Task: Measure flow and transport properties of key contaminant mixtures. Refine theory and numerical models to describe their flow and transport in relevant subsurface environments.

Task: Design, implement and analyze controlled tests of complex contaminant mixtures in highly heterogeneous systems.

Activity MP3: Incorporation of understanding and models for multiphase flow and transport into site assessments and remediation strategies.

Status: Remediation strategies routinely take into account multiphase flow and transport of site-specific contaminant mixtures.

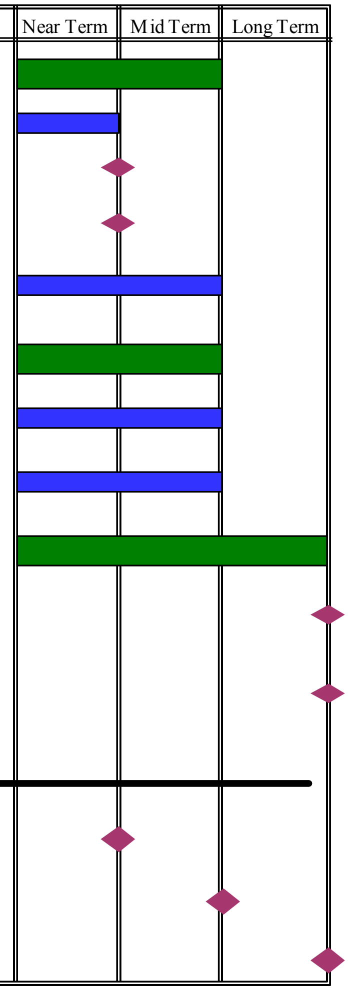
Status: Numerical models are being used to assess uncertainty in flow and transport of complex contaminant mixtures at priority sites (including DOE sites) and to support decisions with regard to remediation and containment strategies.

HIGHLIGHTS OF EXPECTED RESULTS

We can model processes with unstable or preferential flow of aqueous and non-aqueous phases.

We can detect and interpret multiphase flow and transport of complex contaminant mixtures at contaminated sites.

Site assessment models incorporate multiphase flow and transport.



#6 Unstable Processes

	Near Term	Mid Term	Long Term
Activity UP1: Studies of factors influencing unstable flow.			
Task: Identify directions for applying chaos theory in VZ hydrology by (1) reviewing the literature on physical, chemical, and biological processes in which unstable flow occurs; and (2) comparing these processes and conditions with those occurring in the VZ.			
Task: Perform bench-scale and field-scale investigations of factors leading to instability and chaotic-type flow and chemical transport in VZ conditions.			
Status: Criteria have been developed to identify the onset of unstable and/or chaotic-type processes in VZ flow and transport			
Task: To identify conditions for which unstable and/or chaotic-type processes are important, design and perform field-scale infiltration tests with tracers at several sites with VZ contamination in heterogeneous soils and fractured rocks.			
Task: To determine the main diagnostic parameters of chaotic-type flows, develop software that reconstructs the system phase-space from scalar data.			
Activity UP2: Modeling unstable and chaotic flow in the VZ.			
Task: Develop a series of models describing unstable flow phenomena of deterministic chaos in unsaturated fractured rocks.			
Task: Develop a new generation of mathematical and numerical models to describe unstable and chaotic-type flow processes in soils and fractured rocks.			
Task: Implement models of unstable and/or chaotic-type flow into other deterministic and stochastic models used for predicting flow and transport and designing remediation activities.			
HIGHLIGHTS OF EXPECTED RESULTS			
We can identify the onset of chaotic and unstable processes.			
We can determine whether and when chaotic conditions are important at a site.			
Site assessment models incorporate models for chaotic and unstable flow.			

#7 Understanding and Modeling Coupled Systems

	Near Term	Mid Term	Long Term
Activity CP1: Improve existing or develop new databases for processes with coupled GHCB properties.			
Task: Update and check reliability of available databases used in coupled models. Make the reliable databases universally available, with recommendations for usage.			
Activity CP2: Develop cross-disciplinary modeling approaches and implement better models (representations) for key VZ flow and transport processes that cross traditional disciplinary boundaries.			
Status: Better estimation techniques are available to facilitate routine incorporation into process models of different types of GHCB data that have different sampling scales and different spatial variability.			
Status: Coupled processes with the highest priority for understanding VZ fate and transport, and the gaps in understanding them, have been identified.			
Status: Model studies have demonstrated capabilities and limitations of existing coupled models. Procedures for their appropriate use have been codified and are widely disseminated and accepted. Strongly coupled nonlinear phenomena requiring development of new modeling approaches have been identified.			
Task: Use the results from the identification of priority coupled processes and knowledge gaps about them to guide research on sufficiently realistic representations of the highest priority processes.			
Activities CP1 and CP2:			
Status: Realistic representations of the priority coupled processes have been developed, validated in field studies, and implemented in VZ fate and transport models.			
Activity CP3: Develop realistic representations for strongly coupled nonlinear GHCB phenomena. Incorporate adequate models for these phenomena in transport models for VZ contamination sites.			
Status: Models have been formulated for strongly coupled nonlinear GHCB phenomena with high priority for VZ contamination studies. The modeled phenomena may include mechanics of biofilms; multivariate reaction kinetics; saturation and colloid-facilitated transport; and scaling of coupled processes in space and time.			
Status: Constitutive theories and parameter databases for strongly coupled nonlinear GHCB systems have been improved and incorporated into VZ contaminant transport models.			
Status: Models for strongly coupled nonlinear systems have been linked with scaling techniques.			
Status: Mechanical-hydraulic and biochemical-hydraulic prototypes are available for use.			
Status: Models for strongly coupled nonlinear GHCB systems are supported in the PSE			

#7 Understanding and Modeling Couples Systems (cont.)

	Near Term	Mid Term	Long Term
Task: Test proposed models for strongly coupled nonlinear phenomena on synthetic test problems, in small-scale and meso-scale lab experiments, and at field-scale research sites.			
Status: Improved computational algorithms are available for strongly coupled nonlinear GHCB processes.			
Status: Models for strongly coupled nonlinear GHCB systems have been tested in field applications.			
Activities CP1 through CP3:			
Status: Realistic models are available for all coupled GHCB phenomena, including strongly coupled nonlinear processes, that are important to VZ flow and transport. These models cover all important time and space scales, and most of them are available within the PSE.			
Status: Three-dimensional fully coupled heat and multiphase flow and transport models are the norm for decision support.			
HIGHLIGHTS OF EXPECTED RESULTS			
The highest priority coupled GHCB processes have been identified.			
We understand the strengths and weaknesses of existing models.			
Some of the important strongly coupled phenomena can be modeled.			
Process models for important strongly coupled phenomena have been validated and field-tested across spatial and temporal scales.			
Site assessment models incorporate all important coupled GHCB phenomena realistically.			

#8 Combining Processes & Data at Different Scales

	Near Term	Mid Term	Long Term
Activity SC1: Develop simulation tools for VZ systems that provide a hierarchy of constitutive theories and that can simultaneously accommodate multiple processes on different scales.			
Status: A Monte Carlo prototype for massive deterministic simulations of scaling issues has been designed and developed.			
Task: Develop extensions of the massively deterministic Monte Carlo method to include probabilistic specifications of properties and constitutive hypotheses.			
Status: The extended Monte Carlo modeling capability is in use as a testbed for evaluating scaling approaches and for advanced quantification of errors associated with information loss in scaling.			
Status: Scaling is being used to provide quantification of relevant processes by identification of global system variants, such as contaminant trajectories and travel times, non-aqueous mobile phase geometries, cumulative reaction histories over multiple time scales, and subsurface ecosystem dynamics.			
Status: New deterministic and probabilistic/stochastic approaches have been developed to address cross-scale issues that commonly arise in VZ reactive flow and transport.			
Task: Undertake research to understand the time scaling of reaction systems and to solve problems of transients, episodic behavior, and boundary conditions.			
Task: Refine computational techniques for solving hierarchically scaled flow and transport models; test these techniques with meso-scale lab experiments, small scale field experiments, or other types of measurements of coupled GHCB processes.			
Task: Develop scaling methods for flow in generalized (transient and spatially non-uniform) coordinate systems to accommodate processes that vary on multiple spatial and temporal scales.			
Status: Research has provided linkages from constitutive theories and scale of measurement to the quantities of ultimate concern to decision-makers. These linkages are in use for planning and implementing characterization and monitoring activities.			
Status: Models for strongly coupled nonlinear GHCB systems are supported in the PSE.			
Task: Develop links between the scaling methods described above and the methods for uncertainty estimation and reduction in the PSE.			
Status: Research is being done on spatial and temporal scaling in support of source-identification, as well as other inverse problems.			
Status: Strongly transient coupled GHCB processes at applied field sites can be modeled over multiple time horizons.			
Status: Aspects of scaling theory have been unified and completely linked with methods for uncertainty estimation and reduction in the PSE.			
HIGHLIGHTS OF EXPECTED RESULTS			
We can simulate scaling problems of important GHCB phenomena using probabilistic modeling.			
We can measure and model coupled GHCB phenomena across spatial scales.			
Site models incorporate strongly transient and coupled GHCB phenomena for multiple time periods.			
Site models incorporate scaling with estimates of uncertainty, and the models can propagate uncertainty estimates across spatial and temporal scales.			

#9 Estimation & Reduction of Uncertainty

	Near Term	Mid Term	Long Term
Activity UC1: Catalogue, assess, and prioritize R&D needs for addressing the different sources of uncertainty in models of VZ flow and transport.			
Status: State-of-the-art methods of uncertainty estimation and reduction, especially for risk analyses, have been catalogued and assessed.			
Status: Sources of uncertainty in VZ modeling, including choice of conceptual model, geological heterogeneity; parameter values; and initial and dynamic boundary conditions, have been quantified and R&D needs to address them have been prioritized			
Task: Develop and test new theories and methodological approaches for describing and understanding the spatial and temporal structures of naturally occurring heterogeneities and fluctuations. Use advanced geological modeling to capture both flow-sensitive and chemical spatial heterogeneity.			
Status: Uncertainties for flow models of highly heterogeneous porous and fractured media, affected by the fracture-matrix interactions and by film flow in dry formations, have been identified and evaluated.			
Activity UC2: Research to decrease uncertainties in VZ modeling.			
Task: Analyze existing long-term geological, hydrologic, chemical, and biological records to improve conceptual models, reduce their uncertainties, and reduce or quantify the uncertainties in estimates of parameters and boundary conditions used in VZ models.			
Task: Test candidate methods for uncertainty estimation and reduction, and applications of these methods, on synthetic test problems, small-scale and meso-scale lab experiments, and field-scale research sites.			
Task: Evaluate effects of uncertainties for invasive and noninvasive field characterization and monitoring methods with different scales and degrees of resolution.			
Status: Uncertainty estimation and reduction methods resulting from the Activity UC2 tasks with mid-term endpoints (see above) are in use as standard practice at several typical sites with VZ contamination.			
Status: New, more sophisticated and efficient probabilistic approaches to uncertainty estimation and reduction have been developed and tested.			
Status: Uncertainty estimation and reduction methods are in use to predict the value of new data, to optimize the design and operation of characterization and monitoring activities, and to automatically update a model when new data becomes available.			
Task: Develop uncertainty and inverse methods that self-adaptively suggest modified conceptualizations or parameterizations.			
Status: Forward and inverse models accounting for uncertainty are fully integrated into the VZ PSE.			

#9 Estimation & Reduction of Uncertainty (cont.)

	Near Term	Mid Term	Long Term

Activity UC3: Improve computational methods for representing and propagating uncertainties in VZ models.

- **Status:** Numerical algorithms have been improved to increase the efficiency of VZ Monte Carlo simulations.
- **Status:** More realistic treatment of uncertainties caused by surface boundary conditions have been incorporated in VZ models.
- **Status:** Support for uncertainty analyses has been incorporated in VZ PSE.
- **Status:** Methods to display the degree of uncertainty from different sources and in aggregate (processes, coupling, parameters and properties, variability, etc.) have been developed and incorporated in VZ system models. These methods exploit advanced visualization techniques and other sensory (e.g., sound and touch) interactions with models and data.
- **Status:** Users of VZ system models are automatically alerted to possible limitations caused by uncertainty.
- **Task:** Link the analysis of modeling uncertainty with practical problems of a facility designer. Integrate uncertainty estimation and reduction with estimation and reduction of numerical errors. Incorporate these modeling improvements into the VZ PSE.
- **Status:** Uncertainty analysis has been coupled to management models and the VZ PSE to help make decisions concerning characterization, monitoring, and remediation design and operation.

Activities UC1 through UC3:

- **Status:** Uncertainty estimation techniques are incorporated in commonly used biogeochemical models and models of multiphase flow in fractures.
- **Status:** Uncertainty estimation and reduction are standard practice and are in use for characterization, monitoring, remediation, and stewardship decisions.

HIGHLIGHTS OF EXPECTED RESULTS

We have identified and understand the sources of uncertainty for monitoring and modeling vadose zone sites.

We have assessed and catalogued the state-of-the-art methods for estimating and reducing uncertainty.

We have developed and tested new probabilistic approaches for estimating and reducing uncertainty.

We can optimize characterization and monitoring systems to reduce uncertainty, and we can predict the value of additional data for reducing uncertainty.

Site assessment models incorporate techniques for estimating and reducing uncertainty in making decisions on site cleanup and stewardship.

#10 Improving Monitoring Systems

Near Term | Mid Term | Long Term

Activity MON1: Build, catalogue, and update conceptual models for fate and transport of VZ contaminants, using field data on specific contaminant plumes to select and improve models for the catalogue.

- **Status:** At least 2 or 3 conceptual models for fate and transport of particular contaminants, including contaminants of particular interest to DOE, have been built, catalogued, and updated using field data on specific contaminant plumes from DOE sites or other VZ contamination sites.
- **Status:** Field measurements from within and outside the DOE complex have been compiled to provide broad-based technical support for the catalogue of fate and transport models. Characteristic transport distances, chemical controls on attenuation, and hydrologic factors have been determined on a site-specific basis, but these features have been used collectively to update the conceptual models in the catalogue.
- **Status:** Contaminant-specific monitoring needs have been catalogued. Current "standard" monitoring approaches that cannot conceivably update or refine the catalogue of conceptual models for attenuation of a specific contaminant have been identified.

Activity MON2: Coordinate effort to collect long-term monitoring lessons learned from across DOE sites and from other agencies with monitoring experience and expertise.

- **Task:** Use the gathered monitoring data and lessons learned to institutionalize a reflexive and iterative linkage between monitoring and model refinement
- **Task:** Use the gathered monitoring data and lessons learned to (1) condense the catalogue of conceptual models for contaminant attenuation/fate and (2) standardize monitoring approaches.

Activity MON3: Define monitoring requirements and improve/develop monitoring approaches for chemical contaminants.

- **Status:** *In situ* burial or disposal configurations (barrels, drums, boxes, and subsurface structures) can be delineated and distinguished from cultural features and soils.
- **Status:** A cost-effective real-time monitoring and data analysis system has been developed that provides early warning of contaminant discharges to the VZ.
- **Status:** Contaminant-specific monitoring needs have been catalogued.

HIGHLIGHTS OF EXPECTED RESULTS

Several conceptual models for fate and transport (beginning a catalogue) have been validated with field data representing an emerging set of standard monitoring approaches.

Researchers, site operators, regulators and stakeholders can access a catalogue of proven fate and transport models with data sets for priority vadose zone cleanup sites.

Real-time monitoring systems at sites with vadose zone contamination provide early warning of contaminant discharge or movement.

The model catalogue has been condensed and updated, and monitoring approaches have been standardized.

#11 Integrating and Validating Site-Wide Models

Near Term | Mid Term | Long Term

Activity IV1: Improve and test techniques: (1) for estimating model input parameters, including boundary conditions and properties that control flow and transport and, (2) for model integration, through improved measurement system design and/or improved inverse modeling of input parameters.

Task: Develop models of sampling events and instrument response, to be used to improve instrument design, for a variety of invasive and non-invasive methods for characterization and monitoring.

Task: Develop new inversion techniques for estimating the input parameters in models of transient flow and transport processes.

Task: Design and conduct controlled field experiments that distinguish among conceptual models representing different sides of issues in VZ flow and transport.

Status: Improved methods for inverse modeling and estimating probabilistic uncertainty have been tested through meso-scale lab and field-scale experiments.

Status: A highly integrated Shared Vadose Model has been developed, validated, and is being applied. This model is a subset of the PSE in which the value of new data is continually assessed as part of an observation–prediction–decision support (cost analysis) process.

Activity IV2: Develop new tools to test and validate VZ models and techniques, such as inversion methods, for integrating data and estimating key parameters.

Task: Define synthetic test problems and use them to conduct comparative studies of existing techniques for inverse modeling and model validation.

Status: Integrated meso-scale lab and field experiments have been performed to build databases suitable for testing and validating specific models.

Status: A computational test bed to assist in testing and validating models has been incorporated into the VZ PSE.

Status: Support for inverse methods and for decision support simulations has been added to the PSE.

Status: GIS have been linked with, or otherwise functionally incorporated into, the PSE.

Activity IV3: Conduct VZ field experiments to test and refine models and measurement techniques, including advances in instrumentation, tracers, biological properties, and emplacement technologies, as well as mathematical and statistical bases for design.

Status: Models can be tested by comparing model predictions to short-term (and eventually long term) field observations from field test sites and monitoring networks at contamination sites.

Activity IV4: Apply improved methods and tools for integration and validation to real-world problems of managing VZ contamination.

Status: Model testing and validation methods are being applied at major VZ contamination problems, including DOE sites.

Status: Better inverse methods for estimating parameters, boundary conditions, and the uncertainties in these estimates, and better methods for conceptual model validation, have been developed and validated using synthetic problems, experiments, and site data. They are being used to guide characterization and monitoring activities at sites with major VZ contamination problems, including DOE sites.

Activities IV1 through IV4:

Status: Models are an effective bridge to visualize and communicate findings from scientists to policy-makers and stakeholders

HIGHLIGHTS OF EXPECTED RESULTS

We can compare modeling techniques using a standard set of synthetic test problems.

We have models for sampling events and instrument response to improve instrumentation and network design for characterization and modeling.

We can test and validate models and measurement methods in laboratory and field experiments following standard protocols.

Site-wide assessment models are credible to both scientific and public policy communities.

#12 GHCB Data Library and Model Set

	Near Term	Mid Term	Long Term

Activity G1: Build and extend a virtual library of qualified GHCB data.

Task: Tabulate known GHCB features for priority sites with VZ contamination and representative GHCB characteristics.

Status: GHCB virtual library is operational and contains qualified GHCB data for key sites with VZ contamination problems.

Status: Scale parameters are being reported to the GHCB virtual library, as well as measured values and distributions. VZ scientists are comfortable interpreting their measured data using a hierarchical structure of organization that can exist in natural geological environments.

Activity G2: Develop prototypical numerical models that can be used to implement site-specific four-dimensional GHCB framework models incorporating site-relevant GHCB parameters and processes.

Status: Prototype GHBC models are available that run with GHBC virtual library data and/or other suitably structured datasets.

Status: GHBC models and virtual library datasets are adequate to simulate the critical features, parameters and processes for the DOE VZ problem sites and other sites of national interest. The simulations of flow and transport are consistent with all existing qualified data and observations.

HIGHLIGHTS OF EXPECTED RESULTS

A virtual library of qualified GHCB data for priority contaminated sites is available to researchers, site operators, regulators, and the policy communities.

Virtual library data can be run on prototype models that incorporate a GHCB framework.

We can simulate critical features of priority contaminated vadose zone sites using GHCB models and virtual library data.

#13 Sensors, Instrumentation & Emplacement

	Near Term	Mid Term	Long Term
Activity SIE1: Understand the effects of sensor emplacement and apply this understanding to improving sensor emplacement approaches.			
Status: Methods for minimization of emplacement effects, such as microdrilling and coiled tubing, have been demonstrated successfully at important sites of VZ contamination, including DOE sites with high levels of radiological and chemical hazards.			
Status: New drilling techniques for sampling and for sensor emplacement have been developed and tested.			
Task: Develop minimally invasive methods and approaches to correcting for emplacement effects.			
Status: Non-invasive methods or methods to fully correct for emplacement effects are available for all characterization and monitoring needs.			
Activity SIE2: Improve cost-effectiveness of sampling and sensor emplacement techniques.			
Task: To decrease cost and improve spatial resolution, develop sensors that can fit in existing boreholes.			
Status: Deployable prototype sensors are small enough that 10 sensors can fit inside a 2-inch diameter hole.			
Status: Cheaper, smaller, and more robust subsurface location devices have been developed and are available for use.			
Status: Prototype field sensors using alternatives to boreholes are being deployed. These sensors are small enough to support 50 channels of output data in a sensor that fits in a hole the size of a rice grain.			
Status: Injectable sensors and smart sensors are available as off-the-shelf technology. These low-cost sensor technologies provide continuous spectrum coverage, are the size of a soil pore, and require little maintenance.			
Activities SIE1 and SIE2:			
Status: The geology and hydrology of a contaminated site can be characterized at a 10-meter scale throughout the top 50 meters of the subsurface, using methods that have about a one-month turnaround time for processing and interpreting the field measurements.			
Status: The geology and hydrology of a contaminated site can be characterized at a 1-meter scale throughout the top 50 meters of the subsurface, using methods that have about a one-day turnaround time for processing and interpreting the field measurements.			
Status: The geology and hydrology of a contaminated site can be characterized at a 1-meter scale throughout the top 50 meters of the subsurface in real time for most sites.			
HIGHLIGHTS OF EXPECTED RESULTS			
Prototypes of miniaturized sensors are small enough to fit a package of 10 inside a two-inch hole.			
We can characterize the geology and hydrology of a site at a 10-meter scale with one month turn-around.			
Techniques to minimize emplacement effects have been developed and tested.			
Minimally invasive emplacement methods and miniature sensors are available as alternatives to conventional boreholes and instrumentation techniques.			
We can characterize the geology and hydrology of a site at 1-meter scale with a one day turn-around.			
Injectable, smart sensors are available off the shelf; non-invasive methods for measuring key flow and transport properties are available.			
We can characterize the geology and hydrology of a site at 1-meter scale in real-time for most sites.			

#14 Design & Optimization of Measurement Networks

	Near Term	Mid Term	Long Term
Activity ND1: Develop, test, and apply methods for optimizing VZ sensor networks to meet end users' needs for characterization, sitewide assessment, and monitoring information within user-specified constraints of uncertainty and cost.			
Task: Create a numerical lab, combined with highly instrumented field sites, for assessing sensor networks and data value. Define numerical experiments to assess the value of data			
Task: Develop methods to determine the sensitivity of key parameters to sensor network design (and indirectly, cost).			
Task: Determine how design and optimization of sensor networks can reduce uncertainty, taking into account the factors of sensor network cost, data density, and subsurface depth.			
Status: The numerical lab has been upgraded and can now be combined with field data to apply methods for network sensor design to field-scale tests and experiments.			
Task: Develop methods to identify controlling parameters.			
Status: The geophysical method or combination of methods that is most cost-effective for characterizing different geological environments or dynamic processes can be determined.			
Status: Sensitivity to network design can be quickly determined for complex-wide sites.			
Status: Network design and optimization methods are used to convey to end users the cost, data density, and level of investment needed to reduce uncertainty to specific levels.			
HIGHLIGHTS OF EXPECTED RESULTS			
We can access a numerical laboratory linked with instrumented field sites to conduct experiments on characterization/monitoring network design and data value.			
We can use field data in a numerical laboratory to optimize monitoring networks for field-scale experiments.			
We can use network optimization design methods to explain cost-benefit risks and other trade-offs to end users, as part of planning for long-term monitoring and site assessment activities.			
We can quickly determine the location sensitivity and data value for designs of monitoring and characterization networks.			

#15 Facilities for Integrated Field Experiments

	Near Term	Mid Term	Long Term
Activity IFE1: Select, develop, and use national facilities for integrated field experiments aimed at testing VZ research and technology.			
Task: Design and construct IFE support facilities at one or (preferably) more sites representative of priority VZ contamination conditions.			
Status: A first series of shorter-term experiments have been completed.			
Task: Conduct major, long-term integrated field experiments (designed to continue for a decade and longer).			
HIGHLIGHTS OF EXPECTED RESULTS			
Facilities to support IFEs have been constructed at representative sites.			
Results from the first series of short-term IFEs are available.			
Results from major, long-term IFEs are supporting and testing long-term research efforts, improving monitoring systems, and validating integrated assessment models.			

#16 The Problem Solving Environment

Near Term | Mid Term | Long Term

Activity PSE1: Develop and implement a useful first-generation VZ PSE.

Task: Develop the basic PSE structure, including a high-level interface, data structure storage and retrieval approach, simulation engine, and graphical back-end, with a common data structure for modeling and characterization/monitoring.

Task: Implement a limited set of state-of-the-art numerical methods for the first-generation PSE.

Status: A first-generation PSE is implemented, functional, and in use.

Activity PSE2: Extend and update the VZ PSE to provide an increasingly powerful and integrated software framework for studying and solving problems in VZ contamination.

Status: Location-specific databases of parameters have been built and populated.

Status: The PSE has matured to provide users with a wide range of models, including some multi-scale, coupled models.

Status: Models for strongly coupled nonlinear GHCB systems are supported in the VZ PSE.

Status: A computational test bed to assist in testing and validating models has been incorporated into the VZ PSE.

Status: Support for inverse methods and for decision support simulations has been added to the VZ PSE.

Status: Geographical information systems have been linked with, or otherwise functionally incorporated into, the VZ PSE.

Status: Support for uncertainty analyses has been incorporated into the VZ PSE.

Status: Support for a wide range of numerical methods has been incorporated into the PSE.

Status: The VZ PSE has been implemented on state-of-the-art supercomputing environments

Status: The VZ PSE is being used routinely by DOE and other agencies for visualization, analysis, and simulations in support of characterization, monitoring, site assessment, and remediation/stewardship decisions at major sites of VZ contamination.

Status: Realistic models for all coupled GHCB phenomena, including strongly coupled nonlinear processes, that are important to VZ flow and transport are available in the PSE. These models cover all important time and space scales.

Status: The VZ PSE supports state-of-the-art numerics, including full spatial and temporal error estimation with automatic grid refinement.

Status: Support for assessing the value of information has been added to the VZ PSE, including the Shared Vadose Mode

Status: The VZ PSE is broadly accepted and used as a valuable tool to assist all aspects of the development and application of the science: processes, characterization and monitoring, simulation, and prediction.

HIGHLIGHTS OF EXPECTED RESULTS

We can access a shared PSE (software), which includes a common data structure for use in characterization, monitoring, and modeling, as well as a limited set of numerical modeling tools.

An extended PSE, linked to a geographical information system, incorporates a range of numerical methods and provides a computational test bed for validating models.

The vadose zone PSE incorporates realistic models for all coupled GHCB phenomena and state-of-the-art numerics; it supports 'value of information' assessment for monitoring and characterization systems.

#17 Advanced Numerical Algorithms

Near Term | Mid Term | Long Term

Activity NM1: Development and application of better linear and nonlinear solvers to VZ modeling.

Status: Existing state-of-the-art linear and nonlinear solvers have been adapted, improved, and applied to VZ problems.

Status: Linear and nonlinear solvers have been improved to match VZ problems and run in computing environments, such as the VZ PSE.

Activity NM2: Improve approaches to resolve extreme spatial gradients in GHCB properties and processes, such as fingers, sharp fronts, boundaries, and interfaces.

Status: State-of-the-art numerical methods are being applied to modeling spatial gradients of fingers, sharp fronts, boundaries, interfaces, and other extreme-gradient GHCB phenomena.

Status: New and improved numerical methods have been developed and applied for resolving extreme GHCB gradients in both space and time.

Activity NM3: Develop multi-scale mathematical methods and numerics to capture meaningful scales of important GHCB phenomena

Status: Multi-scale mathematical methods and numerics are in use for modeling important GHCB processes, including most linearly coupled, continuous processes.

Status: More sophisticated multi-scale mathematical modeling and numerics have been developed, targeted to non-continuum and chaotic phenomena.

Activity NM4: Develop and apply spatial numerical error estimators and adaptive local (spatial) grid refinement algorithms.

Status: Numerical errors are being estimated in terms of quantities of interest to decision-makers, using spatial numerical error estimators and adaptive, spatially local, algorithms for grid refinement.

Activity NM5: Develop and apply spatial and temporal error estimators and adaptive local grid and time step refinement algorithms for nonreactive systems.

Status: Both spatial and temporal error estimators and grid refinement algorithms (for spatial grid and time steps) are being incorporated in nonreactive flow-and-transport models.

Status: Spatial and temporal error estimators and adaptive local grid and time step refinement have been developed and are being applied for reactive systems in the VZ.

Activity NM6: Determine criteria for acceptable computational errors based on model uncertainties and incorporate algorithms for these criteria in VZ simulation software.

Status: Probabilistic approaches to estimate likely numerical error are available for use in VZ system modeling, instead of maximum error. These probability approaches are being used to estimate mean and variance, as well as other numerical error measures, in terms of quantities of interest to decision makers.

Status: Estimates of maximum, mean, variance, and other numerical error measures in quantities of interest to decision makers are standard practice in modeling VZ systems. Modelers use these estimates adaptively to improve simulation results.

Activities NM1 through NM6:

Status: Support for a wide range of numerical methods has been incorporated in the VZ PSE.

Status: In models of VZ systems, the numerical methods are selected automatically and on an appropriate scale, during computation, to reduce numerical error in decision variables.

HIGHLIGHTS OF EXPECTED RESULTS

Existing state-of-the-art numerical methods have been adapted to address vadose zone problems.

A wide range of numerical methods relevant to vadose zone problems are available.

Site assessment models can automatically select the best numerical method at a spatial and temporal scale to minimize numerical error in decision variables.

#18 High-Powered Computing

	Near Term	Mid Term	Long Term
Activity HPC1: Design, implement, and continue to improve an Environmental Science High-Power Computing capability.			
Task: Build a user community; form an organizing committee.			
Task: Write the proposal for a multi-teraflop (10^{13} to 10^{14} Flops) computing capability, to be associated with the DOE EM Program and/or the Office of Science.			
Status: Proposal for a multi-teraflop computing capability has been submitted to DOE.			
Status: Design of the computing capability has been completed, including its expected future growth in size and capability			
Task: Purchase and install the computing capability at a national laboratory; hire staff.			
Status: HPC capability is in use by VZ researchers on studies of processes, characterization/monitoring, and modeling. It is used to study both lab and field experiments. It is also being used in applied studies for environmental management sites by DOE and other "problem holders."			
Task: Form a committee and write a proposal for the next generation of computing capability.			
Status: The next-generation computing capability is designed, purchased, and installed.			
Status: A next-generation high-power computing capability is in common use for addressing VZ problems.			
Activity HPC2: Build (or transfer from ASCI and others) infrastructure such as desktop visualization, archival storage, and parallel input/output interfaces.			
Activity HPC3: Train the user community for the environmental science high-power computing capability.			
Activity HPC4: Port the VZ PSE to run on the environmental science high-power computing capability.			
HIGHLIGHTS OF EXPECTED RESULTS			
A proposal is submitted to DOE and acquisition of the EHPCC begins.			
First generation EHPCC is in use.			
Second generation EHPCC is in use.			

APPENDIX C. FULL TEXT OF RESEARCH GOALS AS GENERATED BY ROADMAP WORKGROUPS

This appendix lists the research goals as formulated by the three work groups shown in Appendix A. After each research goal, in square brackets is listed the Roadmap Activity in Revision 0.0 to which that goal can be mapped.

Physical Description of Flow and Transport

Near-Term

- Review the state-of-the-practice in DOE for site characterization and remediation, and integrate known models/modules with a sounder physical-chemical basis (state-of-the-science) into DOE flow and transport prediction models and solutions. [Activity PH5 and near-term status point]
- Identify and assess the importance of fluid flow and chemical transport processes and subsurface properties relevant to site characterization, remediation and long-term stewardship (e.g. gravitational, pressure, temperature and chemical gradients). [Activity PH1 and near-term status point]
- Develop methods to quantify spatial variability in flow and transport parameters, fluid properties, thermal properties, biological and chemical reactions. [Activity PH4 near-term status point]
- Develop and implement improved models for evapotranspiration and root water uptake as a function of water stress and other factors. [Activity PH4 near-term task]
- Develop process-hierarchical approaches for describing and modeling controlling processes (e.g., models of increased complexity for flow in structured media, or increasingly sophisticated process-based approximations for gaseous transport or the flow of non-aqueous phase liquids). [Activity PH4 near-term task]

Mid-Term

- Design, implement and analyze controlled laboratory and field experiments to develop the key databases and understanding needed to resolve knowledge gaps in flow and transport processes operative in granular media. [Activity PH2 and mid-term task]
- Develop realistic representations of pore-space geometry of fractured media using geologic, pedologic, and topologic characterization techniques. In parallel, develop and implement improved descriptions of matrix-fracture interactions. [Activity PH3 mid-term task]
- Develop general constitutive relationships for both granular and structured media. [Activity PH3 mid-term task]

- Develop methods for characterizing and propagating physical processes and properties, and their uncertainties, across different scales (governing equations, driving forces, and/or media properties). [Activity PH4 mid-term status point]
- Develop methods for assimilating data from different scales; identify linkages between relevant small-scale processes and properties with larger-scale flow and transport behavior for cases where no simple upscaling is possible. [Activity PH4 mid-term status point]
- Integrate critical elements of chemistry and microbial activity in models for liquid flow and solute transport. [Activity PH5 mid-term task]
- Develop pore network models based upon appropriate equations (e.g. Navier-Stokes), and devise methods for upscaling processes and/or properties from sample to formation scales. [Activity PH3 mid-term task]

Long-Term

- Develop process- and scale-adaptive models for modeling unsaturated flow and transport in different types of porous media. Models should invoke processes at the appropriate scale and employ the corresponding transport and hydraulic properties. [Activity PH4 long-term status point]
- Incorporate solid surface heterogeneity (pore and sample scale), with detailed hydrodynamics into solute transport models (to model opportunity times for reactions, streaming potentials, and other processes or variables). [Activity PH3 long-term status point]
- Incorporate microbiology modules into physical models of solid-gas-liquid environments. [Activity PH4 long-term status point]
- Incorporate solid surface evolution due to biogeochemical reactions (precipitation-dissolution, reduction-oxidation, and other reactions that can change solid-phase geometry and density of exchange sites) into transport models necessary for long time-scale simulations. [Activity PH4 long-term status point]

Measuring Physical Processes and Properties

Near-Term

- Improve methods for measuring moisture content, matric potential, and temperature. [Activity PH6 near-term status point]
- Provide the ability to track a broad waterfront in a 10m X 10m area, at depths up to 100m, to a precision of 10%. [Activity PH7 near-term status point]
- Develop Inverse process of using tracers to estimate fluxes and ages of pore water; propagation of uncertainties to obtain uncertainties in calculated fluxes and ages (2004 - 2025). [Activity PH8 long-term task]

- Use of a variety of tracers for locating contaminants; importance of surface boundary conditions; and point estimates of fluxes and ages (2004 - 2025). [Activity PH8 long-term status point]
- Quantify the relationships among the most likely geophysical methods or combinations of methods that will provide fracture diagnostics. [Activity PH9 near-term task]
- Develop automatic data picking and quality control approaches for crosshole tomographic methods. Also investigate the utility of constrained and joint inversion for improved estimation, and develop stochastic inversion procedures that yield distributions of possible geophysical attributes at each location. Develop new parameter estimation inversion techniques for transient flow and transport processes. [Activity PH11 near-term task]
- Design controlled field experiments distinguishing amongst conceptual models for better assessment of vadose zone flow and transport issues by providing a methodology for model testing, a more formal approach to model formulation, and a larger experience base of observing and measuring vadose zone flow and transport under controlled conditions (2004 - 2025). [Activity IV1 long-term task]
- Develop models of sampling events and instrument response, to be used in improve instrument design, for a wide variety of invasive and non-invasive characterization and monitoring methods. [Activity IV1 near-term task]
- Conduct vadose zone field experiments to test and refine models and measurement techniques. This will include advances in instrumentation, tracers, biological properties, and emplacement technologies as well as mathematical and statistical bases for design. Scale issues, as relative importance of processes to be included in a conceptual model and parameter identification, are critical for field experiment design (2004 - 2025). Develop new model testing and validation tools. [Activities IV3 and IV2]
- Begin to test models by comparing model predictions to short (and eventually long term) observations (2004 - 2025). [Activity IV3 long-term status point]
- Recognize the importance of scale on characterization measurement and incorporate measurement support scale in estimates of hydrological properties and correlation lengths. [Activity PH11 near-term status point]
- Define synthetic test problems and conduct comparative studies of inverse modeling and model validation for these problems. [Activity IV2 near-term task]

Mid-Term

- Resolve a broad waterfront to 5% over a 50m X 50m area. [Activity PH7 mid-term status point]
- Understand at the mechanism of geophysical energy propagation within un- or loosely-consolidated, low pressure, granular porous material at the field tomographic scale, and what are the key influencing factors on the resulting geophysical signature.

We will understand the sensitivity of different geophysical tomographic methods to varied geological conditions, and know if multiple geophysical methods are cost-effective for certain investigations. [Activity PH10 mid-term status point; Activity ND1 mid-term status point]

- Provide estimates of hydrologic properties (e.g. water content, permeability and porosity) and their associated uncertainties and spatial correlation functions using different types of data such as crosshole tomographic. Estimates should be conditioned to direct measurements, and estimation will be made with attention to scale, using hierarchical spatial scale estimation procedures with multi-scaled data. [Activity PH11 mid-term status point]
- Understand which geophysical method or combination of methods is most cost-effective for characterizing different geological environments or dynamic processes. [Activity ND1 mid-term status point]
- Learn how to perform joint and constrained inversions that honor all data, understand how the additional data improves the estimate and decreases the error, and how to incorporate data with different measurement scales in the inversion process correctly. [Activity PH10 mid-term status point]
- Investigate potential of collecting/inverting multi-scaled data to provide information about variabilities as a function of scale. [Activity PH4 mid-term task]
- Develop a quick and reliable way to assess the scale of the contamination problem relative to the scale of the hydrological heterogeneity understanding which technique or acquisition parameters are most appropriate for characterization of the key parameters that control flow and transport. [Activity PH10 mid-term status point]
- Establish methods to incorporate different types of data to assess parameters over different spatial scales. [Activity PH4]
- Attempt to modify the acquisition parameters within a certain type of method to sample different scales of variability and understand how the measurements scale from one level of support to another. [Activity PH4 mid-term task]
- Complete integrated meso-scale laboratory and field experiments to provide databases for specific model testing and validation. [Activity IV2 mid-term status point]
- Establish a computational test bed as part of the Problem Solving Environment (PSE) to assist model testing and validation. [Activity IV2 mid-term status point]
- Improve and apply inverse modeling and probabilistic uncertainty estimation methods to the field and meso-scale laboratory experiments. [Activity IV1 mid-term status point]
- Link GIS (geographical information systems) to the PSE. [Activity IV2 mid-term status point]

- Couple uncertainty analysis to management models and PSE to help make decisions concerning characterization, monitoring, and remediation design and operation. [Activity UC3 mid-term status point]
- Begin applying model testing and validation methods approaches to DOE sites. [Activity IV4 mid-term status point]

Long-Term

- Identify a 3D pulse of water (2m X 2m) to an accuracy of about 2% at depths of up to 100m. [Activity PH7 long-term status point]
- Establish rules of thumb for different environments so quick field tests can determine the category the system under investigation falls into. Utilize the governing petrophysical relationship for that regime with the geophysical data in the estimation routine for first-pass estimations. [Cross-cutting long-term status point for Activities PH10 and PH11]
- Tomographic methods should be able to supply real-time, multi-dimensional (spatially and temporally), automatic interpretations of hydrologic properties or changes in properties due to bacterial modification, environmental remediation, infiltration, and other dynamic processes. (The inversion process should be automatic to provide multi-dimensional, possibly multi-scale, and real-time estimates of hydrologic properties at high resolution). [Cross-cutting long-term status point for Activities PH10 and PH11]
- Establish better inverse methods for parameters, and boundary conditions and models, and their uncertainties. Use as a guide for characterization and monitoring. Test using synthetic problems, experiments, and site data. [Activity IV4 long-term status point]
- Understand how to scale between laboratory- and field-based measurements, and incorporate a variety of differently scaled data to provide an integrated and hierarchical interpretation of hydrological properties. [Activity PH10 long-term status point]
- Develop and apply a highly integrated Shared Vadose Model, a subset of the PSE, where the value of new data is continually assessed as part of an observation–prediction–decision support (cost analysis) process. [Activity IV1 long-term status point]
- Models are finally a "bridge" to communicate findings between scientists and policy-makers. [Cross-cutting long-term status point for Activities IV1 through IV4]

Chemical Properties and Processes

Near-Term

- Be able to determine if various contaminants are present in soils from surface or borehole measurements. May need to couple field results with lab analysis to verify the association. [Activity CH6 near-term status point]
- Be able to delineate in situ burial/disposal configurations (barrels, drums, boxes, and subsurface structures) to distinguish target contaminants from cultural features and soils. [Activity MON3, near-term status point]
- Initiate investigations into the effects of dissolution and precipitation on porosity, pore structure and permeability; initiate studies into nucleation controls that may bias dissolution and/or precipitation to particular pore environments. [Activity CH4]
- Extend solution chemistry models to higher temperatures and ionic strengths (e.g., Pitzer equations) relevant to DOE contamination. [Activity CH1]
- Build conceptual models for attenuation of DOE contaminants on field data of specific contaminant plumes. At least 2 to 3 conceptual models are expected to describe the attenuation of particular contaminants. These should be catalogued/updated in the light of ongoing research (2000 - 2005) [Activity MON1 and near-term status point]
- Improve understanding of kinetic rate mechanisms and effective surface areas; use this understanding to develop improved rate laws. [Activity CH2]
- Determine if significant differences exist for measurement of cation exchange capacity and surface site density between in-situ field measurements of undisturbed samples and laboratory batch measurements involving disturbed media. Determine the validity of using batch Kd measurements to estimate retardation in variably saturated flowing systems. [Activity CH3 and its near-term task]

Mid-Term

- Field measurements from within and outside the DOE complex should be examined and compiled to provide broad-based technical support for the portfolio of “fate” modes. Characteristic transport distances, chemical controls on attenuation, and hydrologic factors will be determined on a site-specific basis but will be used collectively to update the conceptual model portfolio. Two parallel efforts: 1. Cataloguing of contaminant-specific monitoring needs; and 2. Specific identification of "standard" monitoring approaches that cannot conceivably update or refine the cast of conceptual models for the specific contaminant (2005 - 2015). [Activity MON1 and mid-term status point]
- Determine the concentration of the most abundant species within an order of magnitude. [Activity CH6 near-term status point]
- Develop a cost-effective real-time monitoring and data analysis system to provide early warning of contaminant discharges to the vadose zone. [Activity MON3 mid-term status point]

- Investigate mineral reactions in contact with a thin liquid film which may have different properties compared to the bulk fluid and mineral reactions in unsaturated systems having variable gas phase chemistries (e.g., low and high CO2 or O2). [Activity CH5]
- Develop rate laws for glass dissolution and solid solutions that cover more extended conditions typical of natural and contaminant-affected flow fields. Improve models of nucleation processes. [Activity CH4 mid-term endpoint]
- Determine the kinetics (and reversibility) of ion exchange and surface complexation reactions on mineral surfaces and colloids. Resolve the importance of lack of charge conservation in surface complexation models when combined with transport, possibly including streaming potentials in the formulation. [Activity CH3]
- Develop a functional description for porosity/permeability evolution reflecting chemical effects. [Activity CH4 mid-term endpoint]

Long-Term

- Coordinate a DOE-wide effort to collect long-term monitoring lessons learned. There should be enough long-term monitoring data gathered to condense the conceptual model catalogue and to standardize monitoring approaches and to institutionalize a reflexive and iterative linking between monitoring and model refinement (2015 - 2025). [Activity MON2]
- Isolate contaminated volumes and determine the concentration of abundant chemical species within 10 or 20 percent. [Activity CH6 long-term status point]
- Quantify the volume and spatial distribution of resident contaminants at or near source discharge points, for metals, radionuclides, and organics. [Activity CH6 long-term status point]
- Conduct experimental studies to develop appropriate databases of reaction rate constants applicable to refined reaction rate laws. [Activity CH2 long-term status point]
- Couple ion exchange and surface complexation processes to mineral precipitation and dissolution. [Cross-cutting status point for Activities CH1–CH4]

Biological Properties and Processes

Near-Term

- Develop sensors/systems for in situ rate measurements, including improved bioavailability sensors/assays, sample-to-answer analytical systems for community composition and activity; spectroscopy- and synchrotron-based inferences of microbial activity. [Activity B6 and near-term status point]
- Quantify rates of microbial processes affecting inorganics, chelate-inorganic complexes, inorganic complexes, and organic contaminants, and identify factors controlling those rates. [Activity B1 near-term task]

- Understand and predict how contaminant bioavailability affects, and is affected by, microbial processes. [Activity B1 near-term task]
- Develop chemically reactive contact foils and films for in situ rates and/or potential activity. [Activity B6 near-term status point]
- Characterize microbial-mediated corrosion and biodeterioration of materials used to contain DOE contaminants. [Activity B1 near-term task]
- Develop/apply rapid statistical and classification methods for handling large data sets generated from the characterization of microbial communities. [Activity B3 near-term status point]
- Laboratory and modeling of the bio-electric level as a function of different soil types and microbes. [Activity B7 near-term task]

Mid-Term

- Application of in situ bioavailability sensors; sensors/systems for in situ rate measurements and; inexpensive sample-to-answer analytical systems for community composition and activity. [Activity B7 mid-term task and B5 mid-term task]
- Instrumentation developments to detect lower levels of activity and implement these at intermediate and field scale validation tests. [Activity B7 mid-term task]
- Characterize and determine factors governing microbial diversity in the vadose zone. Determine relationships between diversity and community response to contaminants. [Activity B3 mid-term status point]
- Characterize microbial transport in different natural porous media relevant for DOE sites, particularly transport through unsaturated fine and coarse sands and fractured rock, as a function of water saturation and solution chemistry. [Activity B4 mid-term task]
- Improve the conceptual and mathematical characterization of interactions between microorganisms and contaminants (e.g., biodegradation, immobilization, transformation), microbial and physical/chemical processes (coupled processes), and incorporate these equations into reactive transport models. [Activity B1 mid-term task]
- Understand how mixtures of contaminants in DOE wastes affect microbial activity with respect to flow and transport of specific contaminants. Identify conditions when toxicity of radionuclides, metals, or organics prevents removal of readily degradable organic contaminants. Predict the rate of biodegradation of particular contaminants as a function of the type and concentration of other contaminants present. [Activity B2 all]
- Understand the potential roles of siderophore, surfactant, and chelate production by microbial communities in the vadose zone, including the plant root-microbial community interface, on contaminant transformations. [Activity B3 mid-term task]
- Elucidate pore-scale interactions between microorganisms and contaminants, including studies at the microscopic level, and at interfaces (solid/liquid, liquid/gas,

liquid/liquid, solid/gas, and along textural discontinuities) and in biofilms, under undisturbed conditions. [Activity B1 mid-term task]

- Determine the importance of microbial attachment/detachment, biofilms and microbial associations with colloids with respect to contaminant transport and preferential flow. [Activity B1 mid-term task]

Long-Term

- Economical analysis of spatial distribution and temporal dynamics. [Cross-cutting long-term status point for Activities B5-B7]
- Extension of nondestructive joint measurement of biologic, geochemical, physical, and hydrologic properties or processes to intact cores, and possibly the subsurface. [Cross-cutting long-term status point for Activities B5-B7]
- Potential development of proxy measurements for microbiological properties and processes. [Cross-cutting long-term status point for Activities B5-B7]
- Predict in situ rates of microbial biotransformation of contaminants at DOE sites as a function of site and environmental conditions. [Activity B4 long-term status point]
- Incorporate information about the composition of vadose zone microbial communities into pollutant fate and transport models. [Activity B4 long-term status point]
- Predict transport of native and introduced microorganisms at DOE waste sites. [Activity B4 long-term status point]
- Describe and predict the spatial distribution of microbial biomass, activity, and community composition in the vadose zone with respect to contaminant distribution and predict how this distribution is affected by water inputs, contaminant fluxes, and duration of exposure to contaminants. [Activity B3 long-term status point]

Colloidal Properties and Processes

Near-Term

- Consider mobile colloids in sampling and analyses protocols in field and monitoring studies. [Activity COL1]
- Develop new sampling techniques for in-situ measurements of colloidal particles in pore water. [Activity COL1 near-term task]

Mid-Term

- Quantify effect of preferential flow on colloid transport. [Activity COL2 mid-term task]
- Understand relevance of colloid-facilitated transport under transient flow conditions, including wetting-drying and infiltration processes. [Activity COL2 mid-term task]
- Quantify potential for in situ colloid formation and mobilization under conditions relevant for DOE contamination sites, particularly in presence of extreme chemical

conditions that can lead to dissolution and precipitation of soil minerals. [Activity COL2 mid-term task]

- Evaluate specific issues regarding microbial colloids. Research is needed on the effects of changing contaminant flux, nutrient injection during engineered bioremediation, and cell to cell communication (quorem sensing) in biofilms and other cell assemblages, on the production and behavior of microbial colloids. [Activity COL2 mid-term task]
- Characterize colloid-contaminant interactions as a function of solution chemistry and water saturation (micro- and macroscopic level). [Activity COL2 mid-term task]

Long-Term

- Model colloid transport and colloid-facilitated transport in unsaturated soils, sediments, and fractured rocks. [Activity COL3 long-term task]
- Characterize colloid transport in different natural porous media relevant for DOE sites, especially colloidal transport through unsaturated fine and coarse sands and fractured rock, as a function of water saturation and solution chemistry. Colloid interactions with the solid-liquid as well as the liquid-gas interfaces need to be quantified. [Activity COL2 long-term task]
- Improve conceptual and mathematical characterization of colloid-contaminant-soil interactions and colloid-facilitated transport and incorporation into reactive transport models. [Activity COL3 long-term status point]

Multiphase Flow

Near-Term

- Explore the effects of subsurface heterogeneity (physical, chemical, and biological) on multiphase flow and transport processes. [Activity MP1 near-term task]
- Develop upscaling procedures for laboratory-derived multiphase constitutive properties and parameters. [Activity MP1 near-term status point]
- Devise process-based models to describe unstable and preferential flow of aqueous and NAPL phases. [Activity MP1 near-term status point]

Mid-Term

- Measure flow and transport properties of key contaminant mixtures; refine theory and numerical models describing flow and transport of contaminant mixtures; and design, implement and analyze controlled tests of complex contaminant mixtures in highly heterogeneous systems. [Activity MP2]
- Conduct multiphase flow and NAPL transport experiments for representative soils and contaminants to elucidate real-world problems and data limitations. [Activity MP1 mid-term task]

Long-Term

- Refine remediation strategies for site specific contaminant mixtures using numerical models to assess uncertainty in flow and transport of complex contaminant mixtures at DOE sites, and to support decisions with regard to remediation and containment strategies. [Activity MP3]

Chaotic and Unstable Flow

- Review literature related to physical, chemical, and biological processes for which the presence of chaos was established providing comparative analyses of these processes and those occurring in the vadose zone; analyze factors leading to flow and chemical transport instability and chaos based on a series of bench-scale and field investigations. Develop criteria to identify the onset of chaos. [Activity UP1 near-term task]
- Develop a series of models describing phenomena of deterministic chaos in unsaturated fractured rocks. [Activity UP2 near-term task]
- Identify directions of using chaos theory in vadose zone hydrology. [Activity UP1 near-term task]
- Design and perform field-scale infiltration tests with tracers at several DOE sites with heterogeneous soils and fractured rocks to identify conditions for which chaotic processes are important. [Activity UP1 mid-term task]
- Develop a new generation of mathematical and numerical models based on theory of chaotic dynamics to describe unstable, chaotic flow processes in soils and fractured rocks. [Activity UP2 mid-term task]
- Develop software for the determination of main diagnostic parameters of chaos using the reconstruction of the system phase-space from scalar data. [Activity UP1 mid-term task]
- Implement models of unstable, chaotic flow into other deterministic and stochastic models used for predicting flow and transport and designing remediation activities. [Activity UP2 long-term task]

Uncertainty

Near-Term

- Routinely develop petrophysical relationships for different environments, and start to understand how multiple data reduces estimation uncertainly and aids with issues of non-uniqueness between geophysical and hydrological parameters. Become comfortable using stochastic estimation techniques that provide an estimate of the property of interest as well as information about its uncertainty. Develop better estimation techniques to facilitate routine incorporation of different types of data (geological, hydrological, chemical, and biological) that have different sampling scales and different spatial variability. [Activity PH10 near-term task; Activity PH11 near-term status point]

- Assess the state-of-the-art for methods of uncertainty estimation and reduction, especially for risk analyses. [Activity UC1 near-term status point]
- Prioritize and quantify sources of uncertainty, including choice of conceptual model, geologic heterogeneity; parameter values; and initial and dynamic boundary conditions. [Activity UC1 near-term status point]
- Assess uncertainties contributed by geologic heterogeneity in porous media. [Activity UC1 near-term status point]
- Assess uncertainty contributed by dynamic boundary conditions related to weather and climate variability and predictability. [Activity UC1 near-term status point]
- Assess uncertainties contributed by characterization and monitoring methods, including a sample size, sample frequency, etc. [Activity UC1 near-term status point]
- Assess uncertainty contributed by conceptual models of processes, especially overly simplistic or incorrectly scaled process models, and incorrectly coupled processes. [Activity UC1 near-term status point]
- Analyze existing long-term geological, hydrological, chemical, and biological records improving conceptual models and reduce their uncertainties and the uncertainties of parameter and boundary condition estimates. [Activity UC2 near-term task]
- Improve numerical algorithms to increase efficiency of vadose zone Monte Carlo simulations. [Activity UC3 near-term status point]
- Begin testing uncertainty estimation and reduction methods, and their applications, on synthetic test problems, small-scale and meso-scale laboratory experiments, and field scale research sites. [Activity UC2 mid-term task]

Mid-Term

- Establish new theories for describing and understanding the spatial and temporal structures of naturally occurring heterogeneities and fluctuations. Use advanced geologic modeling to capture both flow-sensitive and chemical spatial heterogeneity. [Activity UC1 mid-term task]
- Evaluate uncertainties for flow models of highly heterogeneous porous and fractured media, affected by the fracture-matrix interactions, dry formations, and film flow; add more realistic treatment of uncertainties caused by surface boundary conditions. [Activity UC1 mid-term status point]
- Evaluate effects of uncertainties for invasive and noninvasive field characterization and monitoring methods with different scales and degrees of resolution. [Activity UC2 mid-term task]
- Develop new, more sophisticated and efficient probabilistic approaches to uncertainty estimation and reduction. [Activity UC2 mid-term status point]

- Develop methods to display the degree of uncertainty from different sources and in aggregate (processes, coupling, parameters and properties, variability, etc.). Exploit advanced visualization techniques and other sensual (e.g., sound and touch) interactions with models and data automatically alerting the user to possible limitations caused by uncertainty. [Activity UC3 mid-term status point]
- Use uncertainty estimation and reduction methods to predict the value of new data, to optimize the design and operation of characterization and monitory activities, and to automatically update a model when new data becomes available. [Activity UC2 mid-term status point]
- Implement uncertainty methods at DOE sites to achieve goal of using uncertainty estimation and reduction methods as standard practice. [Activity UC2 mid-term status point]
- Link the modeling uncertainty analysis with practical problems of a facility designer; integrate uncertainty estimation and reduction, with estimation and reduction of numerical errors and; link to Problem Solving Environment. [Activity UC3 mid-term task]

Long-Term

- Incorporate uncertainty in biogeochemical models and models of multiphase flow in fractures (models are in common use). [Cross-cutting long-term status point for Activities UC1 through UC3 and CP1]
- Develop uncertainty and inverse methods that self-adaptively suggest modified conceptualizations or parameterizations. [Activity UC2 long-term task]
- Forward and inverse models accounting for uncertainty are fully integrated. [Activity UC2 long-term status point]
- Uncertainty estimation and reduction is standard practice for characterization, monitoring, remediation and stewardship decisions. [Cross-cutting long-term status point for Activities UC1 through UC3]

Scaling

Near-Term

- Scale parameters should be reported as well as measured values and distributions to a complex-wide database on geological, hydrological, chemical, and biological parameters as a function of geological environment. Vadose zone scientists should also by this time be comfortable interpreting their measured data using a hierarchical structure of organization that can exist in natural geological environments. [Activity PH4 near-term task; Activity G1 near-term status point]
- Begin developing simulation tools that provide a hierarchy of constitutive theories, simultaneously accommodating multiple processes on different scales. [Activity SC1]

- Complete initial design and development of a Monte Carlo prototype for massive deterministic simulations of scaling issues. [Activity SC1 near-term status point]
- Use scaling to provide quantification of relevant processes by identification of global system variants, such as contaminant trajectories and travel-times, non-aqueous mobile phase geometry's, cumulative reaction histories over multiple time scales, and subsurface ecosystem dynamics. [Activity SC1 near-term status point]
- Develop new deterministic and probabilistic/stochastic approaches to address cross-scale issues that commonly arise in vadose zone reactive flow and transport. [Activity SC1 near-term status point]
- Begin research into time scaling of reaction systems and of transient, episodic, boundary value problems. [Activity SC1 task beginning near-term with long-term endpoint]

Mid-Term

- Refine computational techniques for solving hierarchically-scaled flow and transport models; including testing of these techniques to meso-scale laboratory experiments, small scale field experiments, or other types of measurements of geological, hydrological, chemical, and biological processes. [Activity SC1 mid-term task]
- Develop scaling methods for flow in generalized (transient and spatially nonuniform) coordinate systems to accommodate processes that vary on multiple spatiotemporal scales. [Activity SC1 mid-term task]
- Develop extensions of the massively deterministic Monte Carlo method to include probabilistic specifications of properties and constitutive hypotheses. Use it as a testbed for evaluation of scaling approaches and for advanced quantification of errors associated with information loss in scaling. [Activity SC1 mid-term task]
- Conduct research to provide a link between constitutive theories and scale of measurement to the quantities of ultimate concern of decision-makers. Link to characterization and monitoring. [Activity SC1 mid-term status point]
- Improve scaling algorithms and methods. [Activity SC1]
- Begin to develop links to Problem Solving Environment and uncertainty estimation and reduction methods. [Activity SC1 long-term task]

Long-Term

- Broaden research focus to consider spatiotemporal scaling in support of source-identification, (as well as other inverse problems). [Activity SC1 long-term status point]
- Unify aspects of scaling theory, completely linking to Problem Solving Environment, uncertainty estimation and reduction methods. [Activity SC1 long-term status point]
- Have capability to model strongly transient geological, hydrological, chemical, and biological processes over multiple time horizons at applied field sites. [Activity SC1 long-term status point]

Strongly Coupled Systems

Near-Term

- Identify priority coupled process science needs in vadose-zone fate and transport, review the state of the science in constitutive theory for modeling realistically coupled processes, and initiate research on improved representations of coupled processes of immediate importance. [Activity CP2 near-term status point]
- Update and check reliability of available databases used in coupled models. Make databases universally available with recommendations for usage. [Activity CP1 near-term status point]
- Advance models for coupled systems such as: mechanics of biofilms; multivariate reaction kinetics; saturation and colloid-facilitated transport; and scaling of coupled processes in space and time. [Activities CP2 and CP3]
- Develop model studies to demonstrate ability of existing coupled models and recommend procedures for usage. [Activity CP2 near-term status point]

Mid-Term

- Develop and incorporate improved constitutive theories and parameter databases into coupled models; link coupled process models with scaling techniques. [Activity CP3 mid-term status point]
- Mechanical-hydraulic and biochemical-hydraulic prototypes available for use. [Activity CP3 mid-term status point]
- Test coupled models on synthetic test problems, small-scale and meso-scale laboratory experiments, and field scale research sites. [Activity CP3 mid-term task]
- Implement support for strongly coupled models within the Problem Solving Environment. [Activity CP3 mid-term status point]

Long-Term

- Improve computational algorithms for coupled processes. [Activity CP3 long-term status point]
- Test strongly coupled models in field applications. [Activity CP3 long-term status point]
- Realistic models are available for all coupled processes important to vadose zone flow and transport, at all important time and space scales. Most models are available as part of the Problem Solving Environment. [Cross-cutting long-term status point for Activities CP1 through CP3]
- Three-dimensional fully coupled heat and multiphase flow and transport models are the norm for decision support. [Cross-cutting long-term status point for Activities CP1 through CP3]

Understanding the Geological, Hydrologic, Chemical, and Biological Framework

- Tabulate known features for individual sites and start using the geologic/geomorphic understanding to develop 3-dimensional framework models. [Activity G1 mid-term task]
- Develop prototypical numerical models that incorporate the 3-dimensional framework model with the relevant parameters and processes in place. [Activity G2]
- Use models and all existing data and observations to determine the critical features, parameters and process for the sites. In addition, simulations of flow and transport should be consistent with all existing data and observations. [Activity G2 long-term status point]

Sensors and Instrumentation

Near-Term

- Understand the effects of emplacement. [Activity SIE1]
- Demonstrate microdrilling and coiled tubing applied to minimize effects at DOE EM sites. [Activity SIE1 near-term status point]
- Develop new drilling techniques. [Activity SIE1 near-term status point]
- Deploy prototypes in existing boreholes, decreasing cost and improving spatial resolution (goal: 10 sensors, fit in < 2” diameter hole). [Activity SIE2 near-term status point]
- Characterize the geology and hydrology of a contaminated site at the 10m scale throughout the top 50m of the subsurface using methods that have about a one-month turnaround time for processing and interpretation of field measurements. [Near-term status point for both Activities SIE1 and SIE2]

Mid-Term

- Develop minimally invasive methods and begin to correct emplacement effects. [Activity SIE1 mid-term task]
- Develop cheaper smaller robust subsurface location devices. [Activity SIE2 mid-term status point]
- Deploy field prototype using alternatives to boreholes (CPT, new emplacements, microdrilling, autonomous devices, penetrators, injectable microdevices) (goal: 50 channels, rice grain size hole). [Activity SIE2 mid-term status point]
- Characterize the geology and hydrology of a contaminated site to a resolution of 1m and to improve the turnaround time to 1 day, for many field sites. [Mid-term status point for both Activities SIE1 and SIE2]
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Long-Term

- Develop non-invasive methods, or fully correct for emplacement effects; develop injectable sensors and smart sensors that are off the shelf (goal: continuous spectrum, size of a pore in soil hole, low maintenance, and low cost). [Activity SIE2 long-term status point]
- Characterize top 50m of the subsurface to 1m resolution in real time for most sites. [Long-term status point for both Activities SIE1 and SIE2]

Network Design

- Create a numerical laboratory combined with highly instrumented field sites. Define numerical experiments to assess the value of data. [Activity ND1 near-term task]
- Develop methods to determine sensitivity of parameters. [Activity ND1 near-term task]
- Reduction of uncertainty (affected by cost, data density, level). [Activity ND1 near-term task]
- Upgrade numerical laboratory and combine with field data; apply methods to field scale tests and experiments; develop methods to identify controlling parameters. [Activity ND1 mid-term status point]
- Determine sensitivity for complex-wide sites. [Activity ND1 long-term status point]
- Convey to end-users at what cost, data density and level can you reduce uncertainty. [Activity ND1 long-term status point]

Software: Vadose Zone Problem Solving Environment

Near-Term

- Develop the basic PSE structure, including a high-level interface; data structure storage and retrieval approach; simulation engine; and graphical back-end; with a common data structure for modeling and characterization/monitoring. [Activity PSE1 near-term task]
- Implement a limited set of state-of-the-art numerical methods. [Activity PSE1 near-term task]
- Restrict to structured grids. [Activity PSE1 near-term status point]
- Implement on workstations; for forward simulations; and apply on a limited basis. [Activity PSE1 near-term status point]

Mid-Term

- Build/populate the parameter and location-specific databases. [Activity PSE2 mid-term status point]

- Mature to a wide range of models, including some multi-scale, coupled models. [Activity PSE2 mid-term status point]
- Add support for inverse methods, for decision support simulations, for uncertainty analyses, and a wide range of numerical methods. [Activity PSE2 mid-term status point]
- Port to state of the art super computing environments. [Activity PSE2 mid-term status point]
- Apply on a routine basis. [Activity PSE2 mid-term status point]

Long-Term

- Add support for the full range of multi-scale, coupled models, for state-of-the-art numerics, including full spatial and temporal error estimation with automatic grid refinement, and to assess value of information. [Activity PSE2 mid-term and long-term status points]
- Accept and use as a valuable tool to assist all aspects of the development and application of the science: processes, characterization & monitoring, simulation and prediction. [Activity PSE2 long-term status point]

Modern Numerics

Near-Term

- Develop and apply spatial numerical error estimators and adaptive local (spatial) grid refinement algorithms. [Activity NM4]
- Begin estimating numerical error in terms of quantities of interest to decision-makers. [Activity NM4 near-term status point]
- Apply state-of-the art approaches to resolve extreme spatial geological, hydrological, chemical, and biological gradients, such as fingers and sharp fronts, boundaries, and interfaces. [Activity NM2 near-term status point]
- Adapt, improve and apply state-of-the-art linear and nonlinear solvers. [Activity NM1 near-term status point]

Mid-Term

- Develop and apply spatial and temporal error estimators and adaptive local grid and time step refinement algorithms for nonreactive systems. [Activity NM5]
- Complete probabilistic analysis of likely numerical error instead of maximum error and begin estimating mean and variance and other numerical error measures, in terms of quantities of interest to decision-makers. [Activity NM6 mid-term status point]
- Determine criteria for acceptable computational errors based on model uncertainties. [Activity NM6]

- Improve approaches to resolve extreme spatial and temporal gradients, such as fingers and moving sharp fronts, boundaries, and interfaces. [Activity NM2 mid-term status point]
- Develop multi-scale mathematical methods and numerics to capture meaningful scales of important geological, hydrological, chemical, and biological phenomena. [Activity NM3]
- Improve linear and nonlinear solvers to match vadose zone problems and computing environments. [Activity NM1 mid-term status point]

Long-Term

- Develop and apply spatial and temporal error estimators and adaptive local grid and time step refinement for reactive systems. [Activity NM5 mid-term status point]
- Estimating maximum, mean, variance, and other numerical error measures in quantities of interest to decision makers becomes standard practice, and is used adaptively to improve simulation results. [Activity NM6 long-term status point]
- Continue to improve approaches to resolve extreme spatial and temporal gradients, such as fingers, and sharp fronts, boundaries, and interfaces. [NM2]
- Develop more sophisticated multi-scale mathematical modeling and numerics, targeted to non-continuum and chaotic phenomena. [Activity NM3 long-term status point]
- Numerical methods are selected automatically, on an appropriate scale, to obtain reduced numerical error in decision variables. [Cross-cutting long-term status point for NM1 through NM6]
- Continue to develop improved linear and nonlinear solvers. [Activity NM1]

Hardware

Near-Term

- Build a user community; form an organizing committee; write the proposal for a multi-teraflop (1013 to 1014 Flops) computing capability, to be associated with the Environmental Management Program and/or with the Office of Science. [Activity HPC1 near-term task]
- Complete the design of the computing capability, including its expected future growth in size and capability. [Activity HPC1 near-term status point]
- Purchase and install the computing capability at a national laboratory; hire staff; begin building (or transferring from ASCI and others) infrastructure like desktop visualization, archival storage, parallel I/O, etc. Begin training the user community. [Activity HPC1 mid-term task, Activities HPC2 and HPC3]

Mid-Term

- High power computing capability is used by large variety of vadose zone researchers on studies of processes, characterization/monitoring, and modeling; is used to study both laboratory and field experiments; is used in applied studies at DOE environmental management sites. [Activity HPC1 mid-term status point]
- Extend Problem Solving Environment onto the computing capability hardware. [Activity HPC4]
- Form a committee and write a proposal for the next generation of computing capability. Design the machine, purchase and install. [Activity HPC1 mid-term task]

Long-Term

- The next generation computing capability is in common use for vadose zone problems. [Activity HPC1 long-term status point]