Chapter 10
Basic Science

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Overview

The Department of Energy has the responsibility for the cleanup of the nuclear weapons complex, the nation's largest environmental program. The cleanup program "faces many problems that will require new knowledge and fundamental understanding of basic chemical, physical, geological, and biological processes and their relationship to risk" as stated by a committee of the National Research Council [*Building an Effective Environmental Management Science Program*, National Academy Press, 1997, page vii].

In addition, energy and the environment pose major scientific and technological challenges for the 21st century. New technologies for increasing the efficiency of harvesting and utilizing energy resources are essential to the nation's economic competitiveness. At the same time, the quality of life in the United States depends inherently on the environmental impact of energy production and utilization. This *interdependence* of energy use and environmental consequences makes it imperative to develop a better basic scientific understanding of the environment in support of new strategies for minimizing the impact of energy-related activities.

The two major Offices within the Office of Science (SC) that have Environmental Quality R&D responsibilities are the Office of Basic Energy Sciences (BES) and the Office of Biological and Environmental Research (BER). Both of these offices have basic science programs that have been addressing environmental quality issues, in some cases since the beginning of the Atomic Energy Commission. The BER Program mission is to advance environmental and biomedical knowledge connected to energy. Through its support of peer-reviewed research at the national laboratories, universities, and private institutions, the program develops the knowledge needed to identify, understand, and anticipate the long-term health and environmental consequences of energy production, development, and use. The mission of BES is to foster and support fundamental research in the natural sciences and engineering to provide a basis for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use. As part of its mission, BES plans, constructs, and operates major scientific user facilities to serve researchers at universities, national laboratories, and industrial laboratories. In addition, SC's Office of Advanced Scientific Computing Research (ASCR) supports fundamental research in advanced computing research—applied mathematics, computer science, and networking—and operates supercomputer, networking, and related facilities to enable the analysis, modeling, simulation, and prediction of complex phenomena important to the Department of Energy, including its portfolio of environmental science research.

This chapter describes the basic research related to environmental quality that is supported by each of these offices. The chapter is organized by scientific discipline, starting with Biology, Plant Sciences and Bioremediation, and continuing through Chemistry, Computational Science, Engineering, Geosciences, and Global Change (including the multi-disciplinary Climate Change Technology Initiative) to Materials Science. A final section covers major scientific user facilities.

Another important science research program that is directed to environmental cleanup and waste issues for the Department's operations is the Environmental Management Science Program (EMSP). Elements of the EMSP are discussed in other chapters of this report where there are potential applications of the basic research this program supports. Chapter 10 discusses the

fundamental basic science questions addressed by this research and the basic knowledge that is sought through such investigations.

Biology, Plant Sciences and Bioremediation

The biological sciences are coming to the forefront in the Department's environmental research portfolio, thanks to recent fundamental advances in this area, such as the dramatic progress in the genome program, and to a realization that many of DOE's environmental problems cannot be addressed without incorporating the best current research in biology. For example, DOE is supporting fundamental studies to determine the place of microbial bioremediation for dealing with contamination underground that is inaccessible to conventional methods of treatment or that would be too expensive to manage using nonbiological treatment techniques. Likewise, phytoremediation (the use of plants to treat or sequester contaminants) is a very promising technique for dealing with contaminants since plants develop extensive networks of roots in the ground (as much as millions of miles of roots under one acre) that can remediate large underground volumes without constructing an extensive infrastructure as is needed for conventional treatments.

Natural and Accelerated Bioremediation Research

The mission of the Natural and Accelerated Bioremediation Research (NABIR) Program is to provide the scientific understanding needed to make use of natural processes and to develop methods to accelerate these processes for the bioremediation of contaminated subsurface sediments and groundwater at DOE facilities. The program focuses on in situ bioremediation of heavy metals and radionuclides. Scientific understanding will be gained from fundamental laboratory and field research on biotransformation processes, community dynamics and microbial ecology, biomolecular science and engineering, biogeochemical dynamics, and innovative methods for accelerating and assessing *in situ* biogeochemical processes. Field research centers and the supporting infrastructure will facilitate long-term, interdisciplinary research. Computational models will be developed as integrating tools; also they will provide methods for predicting and improving the effectiveness of bioremediation. Additionally, societal implications will be studied to contribute to the appropriate use of bioremediation technologies in safe manner.

The NABIR program provides a framework of basic research in each of seven key areas needed to extend the applicability of bioremediation to many of the environmental problems found at DOE facilities: (1) Biotransformation, (2) Community Dynamics and Microbial Ecology, (3) Biomolecular Sciences and Engineering, (4) Biogeochemical Dynamics, (5) Assessment, (6) Bacterial Transport, and (7) System Engineering, Integration, Prediction and Optimization.

Microbial Genome Program

The Microbial Genome Program focuses on: (1) Genomic sequencing. Microbes are selected for sequencing based on their relevance for energy production, the global cycle, and bioremediation; (2) Microbial diversity. Information is needed on the diversity of microbial species from environments of potential importance to DOE missions, e.g., environments contaminated by high concentrations of toxic metals, and/or radionuclides, likely to contain microbes with metabolic or biochemical properties of potential utility for DOE's missions in waste remediation and clean up, cellulose degradation and energy production; (3) Leveraged sequencing. Strategies are needed that use a previously determined microbial genomic sequence to rapidly, accurately, and cost effectively determine the entire genomic sequence of a related species; (4) Development of improved tools for annotation and analysis of microbial genomic sequence data. This is a critical and fascinating part of the Microbial Genome Project since more than half of the genes identified in newly sequenced microbes are unrelated any genes that have previously been discovered. These new genes represent exciting opportunities for future basic research and potential sources of biological resources to be mined for future use.

Energy Biosciences Program

The Energy Biosciences Program supports mechanistic research on fundamental biological processes related to capture, transformation, storage and utilization of energy. The research focuses on plants and nonmedical microorganisms to form a broad scientific foundation for support of Department of Energy s goals and objectives in energy production, environmental management, and energy conservation. Basic research on plants includes photosynthetic mechanisms and bioenergetics in algae, higher plants, and photosynthetic bacteria; control mechanisms that regulate plant growth and development; fundamental aspects of gene structure, function, and expression; plant cell wall structure, function and synthesis; and mechanisms of transport across membranes. Research supported in these areas seeks to define and understand the biological mechanisms that effectively transduce light energy into chemical energy, to identify the biochemical pathways and genetic regulatory mechanisms that can lead the efficient biosynthesis of potential fuels and petroleum-replacing compounds, and to elucidate the capacity of plants to remediate contaminated environments by transporting and detoxifying toxic substances. The research focus in the microbiological sciences includes the degradation of biopolymers such as lignin and cellulose, anaerobic fermentations, genetic regulation of microbial growth and development, thermophily, e.g., bacterial growth under high temperature, and other phenomena with the potential to impact biological energy production, conversion and conservation. Organisms and processes that offer unique possibilities for research at the interface of biology and the physical, earth and engineering sciences are also studied.

Bioremediation and Phytoremediation

Bioremediation and phytoremediation are a significant focus of basic science funded by the EMSP. The projects in this area can be classified into the following subdisciplines: biodegradation and biotransformation, microbial genetics, microbial transport, plant genetics, plant membrane transport, plant metabolism, biogeochemistry, and bioengineering. In this program element scientists are, for example, studying the genetics and structural biology underlying the mechanisms by which certain plants take up heavy metals, radionuclides and

chlorinated hydrocarbons from contaminated soil and groundwater systems. An early success in this area is the discovery of means to design plants genetically to convert the extremely toxic methylmercury compounds into less hazardous forms. Several projects are studying bacteria that can live in extreme environments such as high radiation fields or high temperatures in order to understand how microorganisms might be used to transform contaminants into less toxic forms. An additional group of projects in the biological sciences is focused on basic understanding of health effects of chemical contaminants and radiation.

Chemistry

Chemistry, with its focus on the molecular level, plays a central role in addressing the needs for fundamental understanding and technology development in both the energy and environmental fields. Understanding environmental processes and consequences requires studying natural systems, rather than focussing exclusively on laboratory models. Natural systems and their complexity pose an enormous, perhaps the ultimate, challenge to chemists, and will provide them with varied and exciting new problems for years to come. In addition, the complexity of the underlying systems and processes often requires multi-disciplinary programs that bridge the interfaces between chemistry and other disciplines. Several major program elements in the chemical sciences support environmental quality R & D. The disciplinary areas within each component are connected to and address the basic research needs of the Department's principal environmental mission goals and objectives.

Heavy Element Chemistry

Developing the fundamental understanding of the underlying chemistry of the actinide elements and separations is important for implementing effective technologies related to pollution prevention, environmental remediation and waste management. The heavy element chemistry program focuses on advancing the knowledge base of the chemical and physical properties of the actinide elements, principally the transuranium elements. A variety of scientific investigations are being pursued within the program, including basic chemical research in near-neutral aqueous solutions, chemistry of aqueous complexing agents, preparative methods for metals and compounds, organometallic chemistry, the chemistry of excited spectroscopic states, thermochemical studies, and characterization in the solid state. The program provides the principal source of new knowledge related to fundamental chemistry of actinide elements with importance to the Department's stewardship responsibilities of these materials, because of their importance to nuclear technology, to the remediation of former weapons production sites, and to applied chemistry efforts in environmental management.

Separations and Analysis

This activity supports basic research to develop better analytical methods for a wide variety of applications in energy processes and environmental sciences, and to improve our understanding of methods for separating mixtures of gases, liquids, solids, and their component molecules, metal cations and anions. Chemical and physical principles that can lead to entirely new methods of analysis are investigated. The research addresses the fundamental molecular level questions underlying separations processes. The program covers a broad spectrum of separations concepts, including membrane processes, extraction under both standard and supercritical conditions, adsorption, chromatography, photo-dissociation, and complexation. The analysis activity supports research on phenomena basic to analytical methods with the goal of improving the sensitivity, reliability, and/or productivity of analytical determinations. Research in this program also encompasses methods for describing turbulent combustion and predicting thermophysical properties of multicomponent systems, where significant energy savings are possible. The science has wide applicability and strong links to the separations and analysis efforts in environmental management.

Catalysis and Chemical Transformations

This program focuses on research related to heterogeneous and homogeneous catalytic systems and to new catalysts for the production of fuels and chemicals, better analytical methods in a wide variety of applications in energy processes and environmental sciences, and new or existing concepts of energy production and storage. Research encompasses chemical aspects of catalysis, both heterogeneous and homogeneous; the chemistry of fossil resources; the conversion of biomass and related cellulosic wastes; and the chemistry of precursors to advanced materials. Creating new, less-energy-demanding routes for the production of basic chemical feedstocks and value-added products is important to energy efficiency. General research that underpins a fundamental understanding of chemical reactivity is also vital, and this, in turn, enables the production of more efficient combustion systems with reduced emissions of pollutants. Understanding of molecular level processes at surfaces, interfaces, and in bulk media are also important to environmental management issues related to pollutant transport and containment.

Photochemistry and Radiation Research

Employing radiation chemistry in environmental remediation requires a basic understanding of radiation chemical processes in complex environmental systems. Fundamental knowledge of how radiolytic reactions occur in heterogeneous systems, including an understanding of how the radiation source, intensity and energy effect reaction rates, mechanisms and product distributions, is required. There is a need to understand the basic mechanisms of advanced oxidation processes, establishing mechanisms of free radical reaction pathways important to remediation, the study of supercritical solvent effects in free radical reactions, and related theoretical and modeling efforts. The program also seeks knowledge of solar photoconversion processes resulting in new, improved systems and production methods. Fundamental concepts of light-induced charge separation at the molecular level are developed for application to photodriven endothermic reactions for the conversion of light energy to chemical energy altering chemical reaction pathways so that high volume industrial intermediates and specialty chemicals can be produced by less polluting processes.

Chemical Physics Research

This program investigates, at the molecular level, chemical reactions in the gas phase, at surfaces, and at interfaces and the relationship between molecular scale phenomena and bulk phenomena. Research activities involve closely-coupled experimental and theoretical efforts. Experimental projects include studies of molecular dynamics, chemical kinetics, spectroscopy, clusters, and surface science. The surface science and clusters research is aimed at providing predictive capability for surface mediated catalysis through provision of explanatory theories relating surface structure to surface mediated chemistry. One of the goals of the chemical physics program is to provide data and techniques for producing or predicting the values of chemical reaction rates to be included in combustion models for predicting the efficiency and emission characteristics of combustion devices and for optimization and control of combustion devices.

Measurement Science

This program supports fundamental research in analytical chemistry with the goal of developing new technologies for improved sensitivity, selectivity, and spatial and temporal resolution of chemical measurements. The Program has provided the basis for major new concepts for instrumentation for environmental characterization (for example, the first demonstration of detection of single atoms, a fundamental advance that led to technology for tracing isotopes in natural and contaminated environments). The program objectives include instrumentation for characterizing environmental chemical composition using spectroscopic techniques, sensors for miniaturized, automated remote monitoring of contaminated environments and technologies for determining the composition of hazardous and radioactive stored wastes.

Chemical Sciences

The chemical sciences are the discipline into which nearly half of the projects funded in the EMSP can be classified. The analytical chemistry and instrumentation component, for example, supports research into laser ablation techniques for characterizing high level wastes and solid waste forms, mass spectrometric research for characterizing hazardous wastes, research into sensors for remote measurement and monitoring of diverse species such as heavy metals, chromium, gamma-ray emitting radioisotopes, and organic contaminants. Actinide chemistry places emphasis on studying the properties of plutonium, americium, curium and the other heavy elements both in high level tank wastes and in subsurface environments. The inorganic and surface chemistry projects include fundamental studies of the chemistry of technetium, a synthetic element found in high concentration in fission products, as well as the study of catalysis of chemical reactions that could determine the long-term behavior of tank wastes or could be used to treat contaminated soils. Separations chemistry also is a major element of the EMSP with several areas of emphasis including design of new chemicals for complexing heavy metals and research into inorganic ion-exchanging materials that could be used to isolate selected contaminants.

Computational Science

In computational science, ASCR supports advanced computing research—applied mathematics, high performance computing, and networking—and operates supercomputer and associated

facilities that are available to researchers 24 hours a day, 365 days a year. The combination of support for fundamental research, computational and networking tools development, and high-performance computing facilities provides scientists with the capabilities to analyze, model, simulate, and—most importantly—predict complex phenomena of importance to the Department of Energy. This capability underpins much of the computational research in support of DOE's environmental missions.

Specific examples of the complex problems relevant to environmental research which are the current focus of computational research in DOE are: climate modeling, including the effects of greenhouse gases on global climate change; the subsurface transport of pollutants; the rational design of new materials to produce, for example, new alloys, superconductors, polymers, and catalysts; theoretical studies of the chemistry of actinides; and the dynamics of multiphase viscous fluids such as oil drilling muds and waste sludges.

Engineering Sciences

In Engineering Research, the goals are to extend the body of knowledge underlying current engineering practice to create new options for improving energy efficiency and to broaden the technical and conceptual knowledge base for solving the engineering problems of energy technologies. The Engineering Research program supports work in three technical areas: (1) mechanical systems including fluid mechanics, heat transfer, and solid mechanics; (2) systems sciences including process control, instrumentation, and intelligent machines and systems; and (3) engineering analysis including nonlinear dynamics, data bases for thermophysical properties, models of combustion processes for engineering applications and foundation of bioprocessing of fuels, and energy related waste and materials. Engineering science in the EMSP includes the study of bubble mechanics and sonification processes for remediation of contamination, robotics and control systems, and on-line diagnostics for waste stream characterization.

Geosciences

In the Department's Geosciences Research program, the goal is fundamental knowledge of the processes that transport, concentrate, emplace, and modify the energy and mineral resources and the byproducts of energy production. The research supports existing energy technologies and strengthens the foundation for the development of future energy technologies. Ultimately, the research impacts control of industrial processes to improve efficiency and reduce pollution, to increase energy supplies, and to lower cost and increase the effectiveness of environmental remediation of polluted sites. The Geosciences Research activity supports basic research in geophysics and geochemistry to improve the level of understanding necessary for advances in and choices among current and emerging energy and environmental technologies. Geochemical research focuses on fundamental understanding of mineral-fluid interactions to provide a better foundation for oil, gas, and geothermal resource recovery and control of contaminants in groundwater flow; new fundamental thermodynamic and physical property information on rocks, minerals, and geologic fluids for resource recovery and contaminant assessment and monitoring; and extending the applicability of isotopic tracer methods for evaluation of natural and human-perturbed processes in the geologic environment. This information, in concert with other

geosciences research, is providing the basis for efforts leading to quantitative predictive capabilities for processes that take place in the Earth's crust.

The EMSP has a major commitment to basic research in the geosciences. This emphasis, present since the start in 1996, has increased in 1999 with the heightened concern with the problems in the subsurface and vadose zone at the Hanford Site. Nearly two-thirds of the projects funded as a result of the subsurface/vadose zone solicitation are in the geosciences. The geochemistry element includes studies of solid/solution geochemistry, colloidal chemistry and transport (a critical concern for example in modeling the potential subsurface transport of plutonium is understanding the extent to which colloidal particles could transport this otherwise generally rather insoluble element), and sorption/desorption geochemistry. The latter area supports research into the factors that influence mobility of contaminants as they interact with the particle surfaces of the subsurface environment. There is a wide range of minerals that need to be studied to allow understanding of the potential mobility of contaminants at DOE cleanup sites and modeling of the transport of these contaminants under various conditions. The research includes studies of clay minerals, quartz, silica, and other naturally-occurring species, as well as materials that are components of tank sludges. The geophysics element supports a range of basic research into techniques for imaging in three dimensions contaminated subsurface environments and underground storage tanks. Among the techniques being studied are high frequency electromagnetic impedence measurement, seismic surface wave tomography and dielectric and nuclear magnetic resonance studies of pore-scale distribution of contaminants. The potential of ground penetrating radar for imaging moisture in the vadose zone is being investigated in this program element. The hydrogeology element has placed an especial emphasis on fundamental properties of dense nonaqueous phase liquids (DNAPLs) in groundwater and unsaturated subsurface environments. The relationship between underground fluid flow and contaminant transport is being investigated both through experimental studies and in research into modeling of these phenomena.

Global Change

The Global Change activities include the process research and modeling efforts needed to (1) improve understanding of factors affecting the Earth's radiant-energy balance; (2) predict accurately any global and regional climate change induced by increasing atmospheric concentrations of greenhouse gases; (3) quantify sources and sinks of energy-related greenhouse gases, especially carbon dioxide; and (4) improve the scientific basis for assessing the potential consequences of climatic changes, including the potential ecological, social, and economic implications of human-induced climatic changes caused by increases in greenhouse gases in the atmosphere and the benefits and costs of alternative response options.

Research is focused on understanding the basic chemical, physical, and biological processes of the Earth's atmosphere, land, and oceans and how these processes may be affected by energy production and use, primarily the emission of carbon dioxide from fossil fuel combustion. A major part of the research is designed to provide the data that will enable an objective assessment of the potential for, and consequences of, global warming. The program is comprehensive with an emphasis on the radiation balance from the surface of the Earth to the top of the atmosphere including the role of clouds and on enhancing the quantitative models necessary to predict possible climate change at the global and regional levels. The Environmental Processes

subprogram is DOE's contribution to the U.S. Global Change Research Program that was codified by Congress in the Global Change Research Act of 1990.

Atmospheric Radiation Measurement Program (ARM)

ARM is a key component of the Department's research strategy to address global climate change. The Program is a direct continuation of DOE's decade-long effort to improve General Circulation Models (GCM) and to provide reliable simulations of regional and long-term climate change in response to increasing greenhouse gases. The ARM Program is a highly focused observational and analytical research effort that collects data for comparison with and improvement of GCMs. ARM operates Cloud and Radiation Testbed facilities in three climatically different locations: the U.S. Southern Great Plains, the tropical western Pacific Ocean, and the North Slope of Alaska. Data are readily available to the researchers in near-real-time. Research objectives are to describe quantitatively the radiation balance from the surface to the top of the atmosphere, to determine the atmospheric characteristics responsible for this balance, to improve the parameterization of the formation and evolution of clouds in climate models, and to operate an experimental testbed for testing process models used in GCMs and for providing satellite ground-truth measurements.

Climate Change Prediction Program

The DOE Climate Change Prediction Program is the next phase in the evolution of DOE's long-standing climate modeling and simulation research agenda. The program is focused on developing climate simulation and prediction models that stay at the leading edge of scientific knowledge and computational technology, testing their performance and applying them to the problem of long-term climate prediction. A unique feature of the program is the establishment of a distributed modeling center involving DOE National Laboratories, the National Center for Atmospheric Research and the nonFederal research community. The program will develop models based on more definitive theoretical foundations and improved computational methods that will run efficiently on future generations of high-performance scientific supercomputers. The intent is to increase dramatically both the accuracy and throughput of computer model-based predictions of the future climate system response to the increased atmospheric concentrations of greenhouse gases.

Climate Change Technology Initiative

The CCTI basic science element focuses on the fundamental science that will enable mitigation of climate change while maintaining a robust National economy.

Eighty-five percent of our Nation's energy results from the burning of fossil fuels, a process that adds carbon to the atmosphere, principally in the form of carbon dioxide. Because of the potential environmental impacts of increases in global atmospheric carbon dioxide, carbon management is an international concern and is a focus of the Climate Change Technology Initiative, a comprehensive research and development program. The Office of Science is well positioned to make significant contributions to this problem, by building on its core programs with novel approaches to make carbon management practical and efficient. Science core programs include research on both carbon and noncarbon energy sources and on both carbon

sequestration and carbon recycling. These activities can serve as the basis for new carbon management science that will lead to the technologies of the future. The theme of efficiency in energy production and use will span the entire range of research activities. Research on carbon energy sources, and their impacts, is a focal point of interagency activity through the U.S. Global Change Research Program (USGCRP). Research on noncarbon energy sources is also a focal point of intra-agency activities and is led by the DOE Office of Energy Efficiency and Renewable Energy. The DOE Office of Science, through activities in both the Basic Energy Sciences (BES) program and the Biological and Environmental Research (BER) program, supports research that underpins both efforts.

Additional science efforts will also have a major effect on a range of scientific disciplines by advancing the state of knowledge and by training students in areas of research that are important to carbon management. These include biochemistry, molecular and cellular biology, structural biology, genome science and ecology. In addition improvements in combustion to reduce carbon emissions require a fundamental understanding in chemical dynamics and theoretical chemistry and physics. Conversion of sunlight to energy requires an understanding in many areas of science, including photochemistry, photosynthesis, metabolism, and solid state physics. The search for increased efficiency in energy production and use requires fundamental knowledge in ceramics, metals, polymers, solid state chemistry, and condensed matter physics for materials that can withstand higher temperatures, have lower coefficients of friction, and are stronger and lighter. Enhanced recovery of fuel resources and of disposal of carbon dioxide requires a fundamental understanding of geometric, structural, and hydrologic properties of reservoirs and of multiphase, nonlinear transport of fluids in porous and fractured structures.

New research efforts supporting advances in low/no carbon energy technologies will provide the knowledge base for the development of advanced technologies to reduce carbon dioxide emissions. Many of the activities will impact the Office of Energy Efficiency and Renewable Energy (EE) and the energy and transportation industry by providing options for increasing efficiency in automobiles by reducing weight; for increasing efficiency in the use of electricity by increasing the efficiency of electric motors and generators with better magnets; for increasing efficiency in the transmission of electricity by using superconductors; and for reducing energy consumption in manufacturing with improved sensors, controls, and processes. Research will provide the knowledge needed to increase the use of renewable resources by understanding the metabolism of carbon dioxide and the metabolic pathways to the production of methane and other biofuels. Other aspects of the research program impact the Office of Fossil Energy (FE) by providing a foundation for effective and safe underground sequestration, new materials, a better understanding of combustion, and improved catalysts.

A climate change technology research and development program must address diverse aspects of the problem including: (1) carbon recycling; (2) improved efficiency in the use of fossil carbon energy sources; (3) new and improved noncarbon energy sources; and (4) carbon dioxide sequestration. The Department has long supported fundamental research in these categories and has particularly strong programs related to the first three. In the Materials Sciences program, research focuses on three areas: high-temperature materials for more efficient combustion, magnetic materials that reduce energy loss during use, and semiconductor materials for solar-energy conversion. In the Chemical Sciences program, research emphasizes atomic and molecular level understanding of chemical processes to enable predictive capability. One goal is

reducing emissions of carbon dioxide through fundamental understanding of the chemistries associated with combustion, catalysis, photochemical energy conversion, electrical energy storage, electrochemical interfaces, and molecular specific separation from complex mixtures. In the Engineering and Geosciences program, research emphasizes carbon dioxide sequestration in subsurface geologic formations. The program will include research to: (1) understand the mechanical stability of porous and fractured reservoirs/aquifers; (2) understand multiphase fluid flow within the aquifers; and (3) understand the geochemical reactivity in relevant conditions. Finally, in the Energy Biosciences program, research emphasizes the biological process of photosynthesis, which is central to global carbon cycling.

Carbon Management Research Program

The Carbon Management Research Program emphasizes decarbonizing fuels and carbon sequestration through several elements. Ongoing CCTI research includes two new Centers for carbon sequestration. CSITE, the DOE Center for Research on Enhancing Carbon Sequestration in Terrestrial Ecosystems, supports research that investigates the enhancement of the natural terrestrial cycle and the potential environmental consequences of enhancing sequestration in the terrestrial ecosystem. The other center, DOCS, the DOE Center for Research on Ocean Carbon Sequestration, investigates enhancing the natural oceanic cycle and the efficacy and impacts of deep carbon dioxide injection. Other ongoing CCTI research includes the sequencing of one marine microorganism and three soil microorganisms that are crucial to affecting the carbon cycle. Other microbes will be selected for sequencing and structural biology will be used to help understand the role of biologically-driven sequestration reactions in the biosphere.

Enhancing the Natural Terrestrial Cycle. Research will identify ways to enhance carbon sequestration of the terrestrial through CO_2 removal from the atmosphere by vegetation and storage in biomass and soils. This includes the development of effective approaches to enhance potential sequestration in part through advances in the fundamental understanding of biological and ecological processes and the formation of soil organic matter in unmanaged and managed terrestrial ecosystems, including wetlands. It also includes efforts to understand ecological consequences of carbon sequestration. The research strategy focuses on those properties and processes of ecosystems for which alteration can offer significant potential for enhancing the net sequestration of carbon. Relevant technical areas of research include: (1) increasing the net fixation of atmospheric carbon dioxide by terrestrial vegetation with emphasis on physiology and rates of photosynthesis of vascular plants, (2) retaining carbon and enhancing the transformation of carbon to soil organic matter; (3) reducing the emission of CO_2 from soils cause by heterotrophic oxidation of soil organic carbon; and (4) increasing the capacity of deserts and degraded lands to sequester carbon.

Carbon Sequestration in the Oceans. The ocean represents a large potential sink for sequestration of anthropogenic CO_2 emissions. Two strategies for enhancing carbon sequestration are (1) the enhancement of the net oceanic uptake from the atmosphere by fertilization of phytoplankton with micro- or macronutrients, and (2) the direct injection of a relatively pure CO_2 stream to ocean depths greater than 1000 m. Sources of CO_2 for direct injection might include power plants, industries or other sources. The long term effectiveness and potential environmental consequences of ocean sequestration by either sequestration strategy are unknown. Research areas relevant to DOE's mission in carbon management include:

(1) environmental consequences of long term ocean fertilization; (2) effectiveness of ocean fertilization on a large scale; (3) environmental consequences of direct injection of CO_2 into the ocean in midwater or deep sea habitats; and (4) effectiveness of direct injection of CO_2 for carbon sequestration.

Sequencing Genomes of Microorganisms for Carbon Management. The Human Genome program has made significant investments in the technology that enables genome sequencing at rates previously unattainable. Capitalizing on these investments, the genomes of microbes that either produce fuels such as methane and hydrogen or that aid in carbon sequestration will be sequenced. This will enable the identification of the key genetic components of the organisms that regulate the production or capture of these gases. New research is being initiated to characterize key reaction pathways or regulatory networks in these microbes following the determination of their DNA sequence. Understanding more fully how the enzymes and organisms operate, we will be able to evaluate their potential use to produce, for example, methane or hydrogen from either fossil fuels or other carbonaceous sources, including biomass or even some waste products. Recently discovered “extremophile” organisms could be used to engineer biological entities that could ingest a feedstock such as methane, sequester the carbon dioxide, and give off hydrogen. Much of the living material responsible for natural carbon dioxide absorption, both on land and at sea, is microbial. Understanding how carbon dioxide “sinks” perform so we can enhance the ongoing natural processes may add powerful new measures to carbon management options.

Materials Science

The DOE Materials Sciences program supports basic research in condensed matter physics, metals and ceramics sciences, and materials chemistry. This research seeks to understand the atomistic basis of materials properties and behavior. Projects are supported in corrosion, metals, ceramics, polymers, glasses, ceramic matrix composites, catalytic materials, nondestructive evaluation, surface science, neutron and x-ray scattering, chemical and physical properties, and new instrumentation. Ultimately the research leads to the development of materials that improve the energy efficiency and environmental acceptability. These material studies affect developments in numerous areas, such as energy efficiency, waste storage and treatment, solar energy conversion, batteries and fuel cells, and stronger, lighter materials.

Materials sciences research seeks and supports basic understanding of materials whose properties are important to environmental quality. Research into the structure of materials enables projections of stability and reliability of vitreous and ceramic materials for the isolation and storage of radioactive wastes. Research in mechanical behavior and radiation effects includes work on the modeling of radiation damage and its effects on fracture toughness and load-bearing capacity of materials for use in high-radiation environments. Research in the area of engineering behavior seeks methods to synthesize new materials for waste storage and impacts efforts to minimize corrosion in hostile environments. The effort in materials chemistry encompasses work that impacts decontamination of surfaces of a wide array of materials used in weapons production activities, from stainless steel to concrete. Finally, fundamental experimental and theoretical research in condensed matter physics seeks understanding at the most fundamental level, from natural formation mechanisms to the role of impurities in material properties. Though

not specifically directed toward environmental quality, all of these programs provide crucial supporting knowledge.

Structure of Materials

This activity supports basic research in the characterization and structure of materials; the relationship of structure to the behavior and performance of materials; predictive theory and modeling; and new materials. This activity provides four complementary electron beam microcharacterization user facilities to characterize localized atomic positions and configurations, chemical gradients, interatomic bonding forces, etc.

Mechanical Behavior and Radiation Effects

This research encompasses studies on the mechanical behavior of materials, including failure and fatigue resistance, fracture toughness and impact resistance, high-temperature strength and dimensional stability, ductility or deformability. These issues are critical to radiation effects, including understanding and modeling of radiation damage and surface modification using ion implantation. These activities relate to energy production and conversion, and radioactive waste storage, through the need for failure resistant materials that perform reliably in the hostile and demanding environments.

Physical Behavior

These activities support basic research in the physical behavior of materials, including aqueous, galvanic, and high-temperature gaseous corrosion and their prevention, phase equilibria and kinetics of reactions in materials in environments under extreme conditions, diffusion and the transport of ions in ceramics and glasses.

Neutron and X-ray Scattering

This activity supports basic research in condensed matter physics that makes use of neutron and x-ray scattering at major DOE user facilities. This research is aimed at a fundamental understanding of the atomic, electronic, and magnetic structure of materials and the effect of structure on the physical properties of materials.

Materials Chemistry

This activity supports basic research on the chemical properties of materials to understand the effect of chemical reactivity on the behavior of materials and to synthesize new chemical compounds and structures from which better materials can be made. The research is aimed at a fundamental understanding of the behavior of novel materials and structures. This activity includes research in solid state chemistry, surface chemistry, polymer chemistry, crystallography, synthetic chemistry, and colloid chemistry, which underpin environmental technologies, including energy efficiency research in fuel cells, batteries, membranes, catalysis, electrochemistry, and solar energy conversion.

Combustion Simulation and Modeling

The program supports research in simulation and modeling, providing detailed understanding of combustion processes to accelerate the development, characterization, and validation of design tools for advanced combustion. Understanding combustion chemistry, fluid dynamics with turbulence, the prediction of combustion device performance, particularly the emission characteristics of combustion devices is relevant to increased energy efficiency.

Materials Science Research

Materials science research is a key component of the EMSP. Nearly a dozen projects are studying the chemical and structural properties of potential waste storage materials. Several of these projects are aimed at understanding the mechanism of radiation effects on glasses that are to be produced in the vitrification of long-lived radioactive wastes. Little is known about the effect of exposure to radiation over long time periods on glassy materials, and these projects are intended to determine the potential for breakdown of glasses through, for example, crystallization or phase separation. Studies are also being carried out on the synthesis and properties of potential crystalline waste storage forms. Several projects are devoted to the study of surfaces to gain understanding of corrosion processes or to determine potential means of cleaning contaminated surfaces.

Scientific User Facilities

The Department of Energy has a long-standing commitment to the operation of major user facilities open to scientists and technologists from the academic, industrial, and government sectors. Indeed the Department's system of scientific user facilities is the largest of its kind in the world.

The most important of these facilities for the environmental field is the William R. Wiley Environmental Molecular Sciences Laboratory (EMSL), located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. As a national scientific user facility, the mission of the EMSL is to provide advanced and unique resources to scientists engaged in research on critical problems in the environmental molecular sciences and to educate young scientists in the molecular sciences to meet the demanding environmental challenges of the future. As a research organization, the EMSL seeks to attain an understanding of the physical, chemical, and biological processes needed to solve critical environmental problems and to advance molecular science in support of the DOE's long-term environmental mission. The EMSL is noteworthy for its unique instrumentation in high field mass spectrometry, high field nuclear magnetic resonance spectrometry, laser spectroscopy, computational chemistry and related fields, and for its emphasis on collaborating with scientists at other institutions in applying this instrumentation to solving environmental problems. EMSL scientists are active in the EMSP, with funding across the range of fields from analytical chemistry through bioremediation to geophysics. These projects emphasize research directed at solving problems in the high level radioactive waste and the subsurface/vadose zone EM need areas.

Other DOE scientific user facilities also provide experimental capabilities that are beyond the scope of those found in laboratories of individual investigators. Synchrotron radiation light

sources, high-flux neutron sources, electron beam microcharacterization centers, and other specialized facilities enable scientists to carry out experiments that could not be done elsewhere. These facilities are planned in collaboration with the scientific community and are constructed and operated in support of forefront research in areas important to the Department as well as to researchers in programs of other agencies and the private sector. These facilities are used by researchers in materials sciences, chemical sciences, earth and geosciences, environmental sciences, structural biology, superconductor technology, and medical research and technology development. The facilities are open to all qualified scientists from academia, industry, and the federal laboratory system whose intention is to publish in the open literature. The four synchrotron light sources are especially important for environmental studies, as they offer capabilities for characterizing the actual chemical form of major contaminants such as plutonium and technetium in unmodified environmental samples. Several EMSP projects are making extensive use of the synchrotrons. One grant funded development of a beam line at the Advanced Photon Source at the Argonne National Laboratory that will be used for a wide range of environmental studies including characterization of subsurface and tank waste samples. The synchrotron light sources will also be used for the study of properties of materials being considered as waste storage forms.