Research Activity: **Geosciences Research**

Division: Chemical Sciences, Geosciences and Biosciences
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Portfolio Description:

This activity supports basic research in rock physics, analytical geochemistry, experimental and theoretical geochemistry, and flow and transport of subsurface fluids. The research seeks to understand how earth properties can be imaged and probed remotely at higher resolution than available with current technology or approaches. It develops analytical methodologies to probe ever smaller mineral domains to track complex reactive processes. It seeks understanding of the controls on complex multiphase reactions among solutions, particles, and surfaces at depth through new experimental methods and computational modeling and simulation of geologically significant processes. It seeks to understand the physics of fluid flow of complex reactive geofluids in highly heterogeneous porous and fractured media at depth. The research is designed to develop understanding of properties to enhance our ability to monitor, measure, and validate ongoing geological processes in the earth. It underlies our ability to track trajectories and rates of chemical and physical processes in the earth. It expands our understanding of the controls on critical geochemical and geophysical processes and provides the foundation for a predictive capability of the changes expected over time. New areas of interest include neutron research in the geosciences that will exploit the BES neutron scattering facilities and nanogeosciences research that challenges our understanding of how traditional measurement techniques of geological materials can accurately reflect geological processes and rates. Natural geosystems with wide ranges of length scales and time scales can be paradigms for how to test and model complex systems and emergent behavior in general.

Unique Aspects:

This activity has an agency-wide mandate to provide new knowledge as the foundation for targeted applications in energy and environmental quality. This activity is pioneering the application of x-ray and neutron scattering to geochemical and geophysical studies. It is the largest supporter of long-term basic research in shallow earth processes in the nation. The objective of this activity is to provide understanding sufficient for imaging, probing, and prediction of shallow earth processes, particularly those related to reactive flow and transport in fractured and porous geological media due to the importance of these problems to multiple Department of Energy (DOE) mission areas. It interacts collaboratively with research programs supported by the Offices of Biological and Environmental Research, Fossil Energy, Environmental Management, and Radioactive Waste Management through support for DOE national laboratory capabilities used by all of these offices. This research program provides enabling understanding for the DOE mission driven programs in environmental cleanup, geothermal energy development, higher-productivity hydrocarbon development, geological sequestration of CO_2 and other energy waste, and long-term monitoring and stewardship of DOE legacy sites. Unique strengths of the program lie in its emphasis on cutting-edge atomic-scale experimental, theoretical, and modeling studies in both geochemistry and geophysics built on the capabilities of national laboratory facilities and over a hundred university research projects.

Relationship to Other Programs:

The Geosciences Program provides 20% ($20M) of the nation's support for individual investigator-driven fundamental research (National Science Foundation (NSF) + DOE ~ $100M) in solid Earth sciences. BES focuses on a narrower range of fundamental issues than NSF (those critical to the DOE mission), particularly in shallow Earth environments, and exceeds NSF support in these areas. DOE user facilities in geosciences, particularly synchrotron x-ray beamlines, are available to all of the geosciences community within the United States.

Significant Accomplishments:

The GSECARS beamline has been built and commissioned (in collaboration with NSF-EAR) as a center for high-resolution analytical geochemistry for the whole Earth sciences community, including multiple DOE applied program users. Geoscience's participation in the BESSRC beamline brings those capabilities to the Earth sciences community as well. Geosciences research projects and a Geosciences workshop on Terrestrial Sequestration of CO_2 were the foundations for identifying research opportunities in this area for the Office of Science and the Office of Fossil Energy. Geosciences workshops have produced broadly applicable publications of Reactive Fluid Flow and Transport Modeling, and enhancing access to Geosciences user facilities which broadly circulate BES interests and approaches to these areas of importance for the DOE. Geosciences investigators have published major review

volumes on Synchrotron Science related to Geosciences, Molecular Modeling applied to Geosciences, Nanophases in the Shallow Earth Environment, Biomineralization, Isotope Geochemistry, Biomineralization and Molecular Geomicrobiology .

Mission Relevance:

The activity contributes to the solution of Earth science-related problems in multiple DOE mission areas by providing a foundation of scientific understanding for applications such as (but not limited to): the potential of geophysical imaging of permeability; reactive fluid flow studies to understand contaminant remediation, or geothermal energy production; and coupled hydrologic-thermal-mechanical-reactive transport modeling to predict repository performance. The DOE applied activities focus on solutions to existing problems in the near-term (0-5 years) but seek fundamental research results as the foundation for their directed research and development efforts in the longer-term, both from the national laboratories and from the university community. In particular, the Geosciences activity provides funding for long-term crosscutting research efforts at national laboratories, which are directly and immediately transferred to the applied programs when needed. The activity also supports the development of research capabilities and communities within both national laboratories and universities that provide manpower for applied programs. The Geosciences activity in BES provides the majority of individual investigator basic research funding for the federal government in areas with the greatest impact on unique DOE missions such as high-resolution Earth imaging and low-temperature, low-pressure geochemical processes in the subsurface.

Scientific Challenges:

Understanding the natural heterogeneity of geochemical and geophysical properties, processes, and rate laws is critical to managing improved production of the Earth's energy resources and safe disposal of energy related wastes. New investigations are needed at the smallest scales studying electronic properties, geochemical reactivity, solute properties, and isotopic distributions in both inorganic and organic systems. Mineral-fluid-microbe systems are also new targets for systematic examination. Understanding pristine natural systems and DOE-specific sites requires improving our capabilities to make and understand high-resolution geochemical and geophysical measurements experimentally and in the field and to model them. Understanding mineral-fluid interactions are key to predicting the fates of contaminants in the environment or predicting nuclear waste-site performance. Improved high-resolution geophysical imaging will underlie new resource recovery, tracking of contaminants, and predicting and tracking repository performance, whether for nuclear or energy-related wastes such as CO_2. Improved imaging and tracking of geochemical processes at the atomic (angstrom) scale using synchrotron x-rays and neutrons is critical for progress in understanding geochemical systems. In addition, new research on high-pressure/high-temperature mineralogical systems will create new opportunities to study and manipulate fundamental mineral and mineral-fluid properties and interactions. Upgrading national laboratory and university investigator experimental, field instrumentation and computational capabilities with new instrumentation and facilities is a continuing challenge. Even with new improved analytical equipment, technical challenges will continue in mastering data-fusion approaches to multiple-technique measurements, such as combined x-ray and neutron analyses or combined seismic-electromagnetic measurements. Computational capabilities driven by the PC-cluster approach with new higher speed chips (3GHz and greater) will enable optimization of clusters for individual molecular dynamics, seismic, electroagnetic, geomechanical, and hydrologic modeling techniques and provide unique support to experimental analysis.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
22,212	20,494	22,345

Performer	Funding Percentage
DOE Laboratories	47 %
Universities	53 %

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

In the near term, geosciences research continues its basic activity in fundamental rock physics, hydrogeology, analytical geochemistry, and theoretical and experimental geochemistry. It continues national laboratory and university projects focusing on understanding the significance of commonly observed natural nanophases and nanoparticles in shallow earth systems. The activity continues working with various groups on investigating uses of neutrons in Geosciences.

In the mid-term, the activity initiates new research efforts on imaging of earth processes under the Chemical Imaging and Mid-range Instrumentation initiatives, with attention devoted both to improved small-scale imaging (geochemistry focus) using x-ray sources, neutron sources, and scanning microscopy, and large-scale imaging (geophysics focus) of physical properties through understanding intrinsic attenuation within seismic and electromagnetic imaging. New high-pressure/high-temperature research activities begin to investigate how physical and chemical properties in the Earth vary with depth and Earth dynamics. The GSECARS and BESSRC at the Advanced Photon Source (APS) begin their second decade as the premier synchrotron user facilities for the earth sciences community, pioneering approaches that can be exported to other facilities such as the National Synchrotron Light Source II (NSLS II).

In the longer term, Geosciences activities will link analytical capabilities with computational capabilities at the nano-, micro- and macro-scales to provide understanding of geochemical processes occurring at natural time and length scales. Geosciences activities will provide robust understanding of what can be measured remotely at depth by geophysical means, and will increase both the depth of current resolution and the resolution at any depths of interest. Geosciences activities will pioneer the use of neutrons to understand geological processes.