Research Activity: Geosciences Research

Division: Chemical Sciences, Geosciences and Biosciences
Primary Contact: Nicholas B. Woodward (Nick.Woodward@science.doe.gov; 301-903-4061)
Team Leader: William S. Millman
Division Director: William H. Kirchhoff

Portfolio Description:

Geochemistry research focuses on advanced investigations of mineral-fluid interactions and developing new methods and techniques for investigating them. It includes studies on rates and mechanisms of reaction, coupled reactive fluid flow, surface geochemistry and geochemical reactivity, and isotopic tracking of mineral-fluid interactions. Improved imaging and tracking of geochemical processes at the atomic (angstrom) to system (kilometer) scale is critical for progress in understanding geochemical systems. Geophysics research focuses on developing an improved understanding of rock, fluid, and fracture physical properties and developing new methods and techniques for investigating them. It includes studies on the surface determination of geologic structures and rock property distributions at depth, improved methods of collection, inversion, and analysis of seismic and electromagnetic data, and identification of geophysical signatures of natural and man-made heterogeneities such as fractures, and fluid flow pathways. All of these studies are focused on improving our resolution in understanding multi-phase heterogeneous natural systems, distributions of chemical, mechanical and physical properties and improved approaches to up-scaling of theoretical predictions and experimental measurements to field-scale systems. The improved resolution comes from improvements in scientific understanding of processes, improved analytical and experimental tools, and improved computational approaches to modeling and algorithm development.

Unique Aspects:

This activity has an agency-wide mandate to provide new knowledge as the foundation for targeted applications in energy and environmental quality. Earth science-related problems are recognized as key elements in seven DOE applied activities (FE - Oil program; FE - Gas program; FE - CO2 sequestration program; NN – Seismology program; EM Science program; RW – Yucca Mountain program; and the EE – Geothermal program). 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 DOE National Laboratory facilities and over a hundred university research projects.

Relationship to Others:

The Geosciences Program provides nearly one third ($21M) of the Nation's support for individual investigator-driven fundamental research (NSF + DOE =$65M) in solid Earth sciences. The BES Geochemistry activities match the size of the Individual Investigator programs in the NSF petrology and geochemistry areas and the BES Geophysics activities match the size of the Individual Investigator programs of the NSF geophysics and NSF hydrology areas, but BES focuses on a narrower range of fundamental issues critical to DOE's mission.

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. One of the program's research projects at APS was selected by that institution as one of its top five studies done in 2000. Geosciences research projects and a Geosciences workshop on Terrestrial Sequestration of CO_2 were the foundations for the DOE Carbon Sequestration Roadmap in the area of geological sequestration and remain the basis for identifying research opportunities in this area for the Office of Science and the Office of Fossil Energy.

Importance/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 seismic imaging for reservoir definition or explosion detection, 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 applied activities all seek fundamental research results as the foundations for their directed research and development efforts, 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. An example is the EM Science Program, which derived over 25% of its subsurface contamination focus area investigators from projects initially supported by BES Geosciences. 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.

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 (1.8GHz and greater) will enable optimization of clusters for individual molecular dynamics, seismic, electromagnetic, geomechanical and hydrologic modeling techniques and provide unique support to experimental analysis.

Funding Summary:

Dollars in Thousands

FY 2000	**FY 2001**	**FY 2002**
$21,615	$ 21,419	$21,387

Performer	**Funding Percentage**
DOE Laboratories	52.0%
Universities	44.0%
Other	4.0%

Projected Evolution:

In the near term, geosciences research continues its basic activity in fundamental geochemistry and geophysics, and research related to CO_2 sequestration. It continues a multi-laboratory project led by Oak Ridge on Chemical Interactions at the Metal Oxide Aqueous Solution Interface in collaboration with the NSF funded NIRT university-based program. Two short courses will be held in the Geosciences Education Initiative series, (Stable Isotope Geochemistry, November 2001; Nanophases in the Environment, December 2001). The activity works with the Neutrons for Geosciences group at LANL to develop a research plan for critical Geosciences experiments. The activity works with NSF-Earth Sciences to develop a collaborative approach on fundamental science projects to be conducted at the NSF Earthscope – Plate Boundary Observatory. Planning begun on upgrades to national laboratory experimental and computational facilities.

In the mid-term, the activity initiates new research efforts Imaging of the Earth 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. University facilities program discussions begin. 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 at the APS reaches its full operational potential as a national user facility for the Geosciences Community.

In the longer term (3-5 years), collaboration begins with NSF-Earthscope, requiring both facilities support and increased funding for critical scientific investigations. The Neutrons for Geosciences efforts reach their goals of enabling new approaches and new discoveries in the geosciences. There is a broadly increased usage of neutrons within the geosciences – which similarly requires both facility support and funding for scientific investigations. Major upgrades/rebuilding efforts will be required at beamlines supported by the program at the NSLS, and at geochemistry laboratories at ORNL, LANL, and LBNL.

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