

Geosciences Research

Portfolio Description

This activity supports basic experimental and theoretical research in geochemistry and geophysics. Geochemical research emphasizes fundamental understanding of geochemical processes and reaction rates, focusing on aqueous solution chemistry, mineral-fluid interactions, and isotopic distributions and migration in natural systems. Geophysical research focuses on new approaches to understand the subsurface physical properties of fluids, rocks, and minerals and develops techniques for determining such properties at a distance; it seeks fundamental understanding of wave propagation physics in complex media and the fluid dynamics of complex fluids through porous and fractured subsurface rock units. Application of x-ray and neutron scattering using BES facilities plays a key role in the geochemical and geophysical studies within this activity. The activity also emphasizes incorporating physical and chemical understanding of geological processes into multiscale computational modeling. Capital equipment funding is provided for items such as x-ray and neutron scattering end stations at BES facilities for environmental samples and for augmenting experimental, field, and computational capabilities.

Unique Aspects

The activity contributes to the solution of Earth Science-related problems in multiple DOE mission areas by providing a foundation of scientific understanding for them. Examples of these applications include (but are not limited to): the potential for geophysical imaging of permeability; reactive fluid flow studies to understand contaminant transport and remediation, and geothermal energy production; and coupled hydrologic-thermal-mechanical-reactive transport modeling to predict geological 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.

Relationship to Other 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. BES focuses on a narrower range of fundamental issues than NSF. DOE user facilities in geosciences, particularly synchrotron x-ray beamlines, are available to all of the geosciences community within the United States. BES research activities focus primarily upon the physical and chemical properties of geo-systems with a cognizance of critical biological interactions. This contrasts with research programs in the Office of Biological and Environmental Research (BER), which primarily focus on biological interactions with the physical and chemical properties of geo-systems, and on DOE site-specific issues. The BES geosciences activity is closely coordinated with applied programs focused on geological CO₂ sequestration within the Office of Fossil Energy (FE) and geothermal energy within the Office of Energy Efficiency and Renewable Energy (EERE).

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. The Geosciences activity also supports BESSRC at the Advanced Photon Source (APS) and X26a at the National Synchrotron Light Source (NSLS). Geosciences supported investigators have been selected in a highly competitive process to design and build one of six facility-supported beamlines at the NSLS-II facility at Brookhaven National Laboratory. Geosciences research projects, unique BES supported laboratory facilities, and BES funded workshops on Basic Research Needs for Geosciences and in topical areas are the foundations for identifying research opportunities for research and development integration activities between the Office of Science and the applied program offices. Recent Geosciences workshops have produced broadly applicable publications on geosciences user facilities, reactive fluid flow and transport modeling, and geophysical processes and properties that can be imaged for environmental applications. These documents promote BES activities to the science community in areas of importance for the DOE and publicize DOE research interests to the broader science community. Geosciences investigators led a National Academy of Sciences study of grand challenges for the earth sciences which was published in March 2008 as *Origin and Evolution of Earth: Research Questions for a Changing Planet*. Investigators sponsored by this activity 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, Isotopic Geochemistry, and Molecular Geomicrobiology, and have published a number of recent textbooks.

Mission Relevance

This activity provides the basic research in geosciences that underpins the nation's strategy for understanding and mitigating the terrestrial impacts of energy technologies and thus is relevant to the DOE mission in several ways. It develops the fundamental understanding of geological processes relevant to geological disposal options for byproducts from multiple energy technologies. Knowledge of subsurface geochemical processes is essential to determining the fate and transport properties of harmful elements from possible nuclear or other waste releases. Geophysical imaging methods are needed to measure and monitor subsurface reservoirs for hydrocarbon production or for carbon dioxide storage resulting from large-scale carbon sequestration schemes.

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. 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. New investigations are needed at the smallest scales to study electronic properties, geochemical reactivity, solute properties, and isotopic distributions in both inorganic and organic systems. Facilities such as the Linac Coherent Light Source (LCLS) will provide unique capabilities for Geosciences investigators to probe natural reactivity processes at ultrafast times to provide a new paradigm for understanding geological reaction rates. Mineral-fluid-biological 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 surface-particle-fluid

interactions is the 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 CO₂). 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, electromagnetic, geomechanical, and hydrologic modeling techniques and provide unique support to experimental analysis.

Projected Evolution

In the near term, geosciences research continues its basic activity in fundamental rock physics, fluid flow, and analytical, 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 and how they contribute to mineral-fluid interactions. The activity continues working with various groups on investigating uses of neutron imaging in Geosciences.

In the mid-term, the activity initiates new research efforts on imaging of earth processes 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 energy waste storage options will require high-resolution monitoring and verification at a new level of sophistication. 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 designing other facilities such as the National Synchrotron Light Source II (NSLS II). They will expand research efforts in nanogeosciences to understand the role of nanophases in geological systems and efforts on understanding the geophysical and geochemical challenges of predicting the fate and transport of CO₂ as sequestration in deep geological formations is tested as a technology option to mitigate greenhouse gas emissions.

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.