Geosciences

Portfolio Description

The geosciences program supports basic research in geology, geochemistry, and geophysics. Geochemical research emphasizes fundamental mechanistic understanding of reactions in earth materials including aqueous solutions, minerals, and organic matter, with particular emphasis on interfacial systems. Geophysical research focuses on the coupled thermo-hydrological-mechanical-chemical (THMC) properties of earth materials across multiple length and time scales with particular emphasis on brittle failure and fracture evolution. Geological research is focused on the development and implementation of methods to investigate long-time-scale geological processes with the highest possible accuracy and at the finest possible time resolution, as well as on fundamental understanding of the occurrence, extraction, and depletion of critical energy materials in the earth's subsurface.

Scientific Challenges

Understanding the natural heterogeneity of geochemical and geophysical properties and processes 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 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 reactivity, solute properties, and isotopic distributions in geological materials. 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 and put them into the context of long-time-scale geological processes. Understanding mineral surface-particle-fluid interactions is key to predicting the fates of contaminants in the environment or predicting nuclear waste-site performance. Improved high-resolution geophysical process modeling 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). 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 probes. Computational capabilities enabled by new high-performance computing architectures will be important contributors to molecular and geomechanical modeling techniques and will provide unique support to experimental analysis.

Projected Evolution

In the near term, geosciences research continues its focus on geomaterial properties; hydrogeomechanical modeling; and analytical, theoretical, and experimental geochemistry. It continues national laboratory and university projects focusing on understanding, at the finest possible resolution, the significance of fluid-rock interactions and how they contribute to mineral-fluid reactivity and chemical migration. Program activities will continue to investigate uses of synchrotron and neutron imaging in geosciences.

In the mid-term, the activity initiates research efforts aimed at discovering new earth processes. This discovery focuses on both small-scale, high-frequency processes (using pulsed x-rays, neutron sources, high-resolution mass spectrometry, and computational molecular modeling) and large-scale, long-time processes (using THMC modeling and imaging of the dynamic response of earth materials to perturbations). Activities continue to drive improvements in subsurface access and in manipulation of processes to optimize subsurface response.

In the longer term, Geosciences activities will link analytical capabilities with computational capabilities at the micro-, meso-, and macro-scales to provide understanding of geological processes occurring at natural time and length scales and to test this understanding with increasingly accurate and fine-scale indicators of geologic history. Geosciences activities will provide robust understanding of the connection between chemical and mechanical coupling in earth materials across multiple length and time scales.

The BES Geosciences program does not fund research focused on single application areas such as, for example, CO_2 sequestration or geothermal energy production, or on topics such as signal processing and applied geophysics. Investigators proposing research in these areas should contact the appropriate technology office.

Significant Accomplishments

Over the last two decades, major accomplishments have been made in aqueous solution thermodynamics, nanogeoscience, high-resolution isotope geochemistry, reactive transport modeling, geomaterials rheology and stress response, and fracture network dynamics. Some recent examples include:

- Research on redox-driven interfacial processes occurring in highly insoluble subsurface iron oxides has revealed an unexpected highly dynamic, rapidly overturning interface driven by transfer of ferrous iron from solution into the predominantly ferric iron oxide. Such processes have implications for contaminant transport, which is often governed by redox transformations, and also for the ability of iron oxides to act as records of geologic processes over long time scales.
- Imaging of crystal growth dynamics on low-temperature, insoluble oxides and biominerals has led to the realization that crystallization proceeds not only via atom-by-atom processes but also by aggregation of preformed crystallites of the dimensions of nanometers. This work has implications for the design of toughened, fracture resistant materials.
- Construction of the first nuclear magnetic resonance probes capable of operating at gigapascal (10,000 atmosphere) pressures. This work gives new mechanistic insights into aqueous reaction mechanisms by subjecting reacting species to high pressures.
- Development of the first secondary-ion mass spectrometry capability for resolving isotope variations at 1 micron resolution. This work allows reconstruction of unprecedented detail in the chemical evolution of shales from burial to lithification and hydrocarbon generation.
- Development of new techniques for dating the evolution of fracture networks forming from dehydration and hydrocarbon release during sedimentary basin evolution. This work provides insight into pathways of hydrocarbon migration and accumulation.

Unique Aspects

Society and industry rely on the earth to provide both energy resources and the raw materials to synthesize energy production systems. As the easily-extracted energy resources are consumed, increasing demands are placed on subsurface science to provide novel ways of accessing new types of resources and to do this in a high-yield, safe, and cost-effective manner. The earth must also be the ultimate repository of energy wastes. Intelligent waste management strategies rely on understanding, and planning for, a myriad of possible THMC processes, operating in the earth's crust on a wide range of time scales, many of which have not yet even been identified. Program activities provide basic knowledge needed for the solution of earth science-related problems in multiple DOE mission areas.

The defining aspects of the program are based on DOE capabilities in high performance computing, x-ray science, and neutron science. The BES Geosciences program plays a pioneering role in two major areas of geoscience research:

1) Molecular geochemistry, combining x-ray and neutron scattering observations with computational chemistry to reveal mineral-water interfacial structure and dynamics at the molecular level.
2) Geophysical process imaging, combining inversion of seismic, electromagnetic, and remote sensing data with THMC forward modeling codes to discover new geophysical processes operating in the shallow crust.

These areas define the BES Geosciences program relative to other federal funding agencies supporting geosciences research, such as the National Science Foundation and the United States Geological Survey. Examples of applications of these focus areas include (but are not limited to): (i) fundamental reaction mechanisms at mineral-water interfaces at the atomic/molecular level to better understand contaminant migration; (ii) reactive fluid-flow studies to better understand hydrocarbon transport, contaminant transport and remediation, and geothermal energy production; (iii) coupled THMC reactive transport modeling to increase the reliability of geological repository performance assessments.

Mission Relevance

Basic research in geosciences underpins knowledge behind improved access to the earth's subsurface and fosters a better understanding of the terrestrial impacts and limitations of energy technologies. This research informs the nation's strategy for optimizing access and mitigating impacts in a safe and cost-effective manner.

Performance assessments of energy production and disposal systems cannot be tested with any usual engineering approach. They have to rely upon conceptual and computational predictions of those systems over long temporal (decades to centuries to millennia) and spatial (kilometers) scales, based on geological observations. BES Geosciences program activities develop a fundamental understanding of geological processes relevant to energy materials production and to geological disposal options for byproducts from multiple energy technologies.

This new knowledge is critical to monitoring, verification, and accounting metrics associated with the development of new energy technologies, serving as a foundation for consent-based energy extraction and waste disposal activities. Knowledge of subsurface geochemical processes, operating both now and in the geologic past, is essential to determining the fate and transport properties of harmful elements from possible nuclear or other waste releases and to assessing the distribution and availability of critical energy materials in the earth's subsurface. Geophysical modeling methods are needed to predict the response of subsurface reservoirs for energy materials extraction and waste storage.

Relationship to Other Programs

- With its focus on molecular interfacial geochemistry, the Geosciences program has strong connections to other BES Chemical Sciences, Geosciences, and Biosciences Division programs, including Condensed Phase and Interfacial Molecular Science, Chemical Theory and Computation, Heavy Element Chemistry, Solar Photochemistry, and Catalysis. In interactions with these programs, Geoscience provides expertise on interfacial processes occurring in chemically complex earth-abundant natural phases and receives input on innovative new theoretical and computational techniques perfected and validated on more idealized synthetic systems.
- Geosciences researchers also participate in Energy Frontier Research Centers.
- DOE user facilities, particularly synchrotron x-ray beamlines, are available to all of the geosciences community within the United States. BES research activities provide examples of innovative use of these user facilities focused on physical and chemical properties of geological systems.
- BES Geosciences activities are coordinated with applied programs within the Office of Fossil Energy (FE) and on Geothermal Energy within the Office of Energy Efficiency and Renewable Energy (EERE-GTO), and other DOE mission programs such as Environmental Management (EM) and Legacy Management. The BES program provides fundamental understanding of geochemical reactivity, the coupling of subsurface flow to geomechanical behavior of earth materials, and high-resolution geophysical process modeling that provides the foundation for predicting the long-term reliability of geological CO_2 sequestration (FE), devising approaches for utilizing geothermal energy (EERE-GTO), and understanding contaminant fate and transport in subsurface environments (EM).[1]

[1] See Basic Research Needs for Geosciences (https://science.energy.gov/~/media/bes/pdf/reports/files/Basic_Research_Needs_for_Geosciences_rpt.pdf) and Subsurface Science, Technology, and Engineering Research and Development (SubTER) Roundtable Report (https://science.energy.gov/~/media/bes/pdf/reports/2015/Controlling_Subsurface_Fractures_and_Fluid_Flow_rpt.pdf)