Geological Research

CHEMIN: A Miniaturized X-Ray Diffraction and X-Ray Fluorescence Instrument

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We have designed a miniature instrument, CHEMIN, which simultaneously uses x-ray fluorescence to identify the elemental chemistry of a sample and x-ray diffraction to identify its mineralogy, or crystalline structure. Originally developed for space travel to Mars, CHEMIN has the potential to serve many uses on Earth, including as a portable field instrument or as part of a robot that analyzes contaminants in hazardous areas. This project is discussed in detail in the Research Highlights section.

Modeling Diffraction Effects from Disordered Materials Using the Rietveld Method

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Clay minerals (such as kaolinite, illite, chlorite, and montmorillonite) have strong intralayer bonding, but the bonding between the individual layers is weaker, leading to considerable disorder in layer stacking. X-ray diffraction (XRD) is the most common technique used to analyze the crystal structures of clay minerals. Unfortunately, the preferred method for interpreting the XRD data, the Rietveld method, cannot be used to model diffraction effects from disordered materials, such as the clay minerals described above. To modify the Rietveld method so that we can model clay minerals, we collaborated with R. Reynolds of Dartmouth College, who is modeling the XRD phenomena from disordered clay minerals. In Reynolds' model of intensity diffracted by disordered crystals, the interference function treats the indices of the diffracting planes as continuous variables, and diffracted intensity is calculated and summed throughout reciprocal space.

As a result of this collaboration, we can now model disorder in the mica/smectite mineral group, and we have developed new disorder theories for the kaolin minerals. We modified our code to compute in any symmetry, and it produces excellent agreement between experimental and calculated diffraction patterns for many clay minerals. We have also formulated a model to incorporate the effects of random X-Y displacements. We have completed the disorder model for the major clay minerals, and derivatives for all disorder parameters have been coded to allow refinement of these parameters rather than simply modeling their effects. This is a requirement for including disorder effects in a Rietveld refinement, and it has never before been accomplished. We will produce a FORTRAN code that embodies the theory of diffraction from both ordered and disordered material, and the code will be incorporated into existing Rietveld refinement programs to allow explicit analysis of samples containing clay minerals.

Geothermal Exploration/ Resource Evaluation

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In this project, we conduct major- and trace-element chemical analyses of geothermal waters, gases, rocks, and veins; geothermal/geochemical exploration; and modeling for various DOE-funded geothermal research projects. We also participate in multiagency investigations of injection-well scaling, long-term geochemical changes, regional recharge, and fumarole/dead zone growth in the Dixie Valley, Nevada, geothermal system. Our studies in the Geysers-Clear Lake region focus on the changes in activity at Anderson Hot Springs and the environmental concerns at Sulphur Bank Mine. In addition, we are studying hydrothermal illite dating and hydrothermal breccia formation in the Awibenkok geothermal core from Indonesia. We recently installed a new Inductively-Coupled Plasma-Mass Spectrometer to improve detection limits and shorten analysis times for various samples.

A Geoscience Approach to Rock-Solid Concrete

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The alkali-silica reaction (ASR) is one of the leading causes of premature degradation in concrete. We recently developed a geochemical staining method, ASR Detect™, which reveals the gel that is a product of this reaction. We are using the method to help understand the degradation process, including the possible role of microbial activity, with concrete structures in the field. This project is discussed in detail in the Research Highlights section.

Measuring Total Soil Carbon with Laser-Induced Breakdown Spectroscopy

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We are testing a new spectroscopic method for measuring total soil carbon. This technique, based on laser-induced breakdown spectroscopy, can provide rapid and efficient measurements in agricultural and forest soils. Such information is vital if we are to mitigate overall U.S. carbon emissions. This project is discussed in detail in Research Highlights.

Uncertainty and Upscaling in Porous Media Flow

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The processes associated with fluid flow through porous rocks and sediments are at the core of problems in groundwater flow, contaminant migration, and petroleum production. Rather than model these processes using Monte Carlo techniques, we are developing an approach based on partial differential equations. This project is discussed in detail in the Research Highlights section.