



the **ENERGY** lab

R&D FACTS

Geological & Environmental Systems

NETL's Fluid Chemistry Analysis Capacity

Background

Establishing the geochemistry of surface and ground waters requires an arsenal of techniques devoted to determining the constituents these waters contain and the environment in which they exist. Many standard techniques have been developed over the years, and new ones continue to be explored as more complex matrices and harsher environments are encountered. Deep geologic storage of carbon dioxide and the development of unconventional oil and gas resources are two areas of current concern where the study of geochemical processes is challenging due to the complex nature of the natural samples, and where routine analytical techniques are being pushed to their limits. The facilities at NETL include both conventional and cutting-edge instrumentation and the application of conventional techniques, as well as the development of new analytical strategies.

Goals and Objectives

Fluid chemistry analysis supports objectives in both the CO₂ storage and unconventional resources project areas. In the CO₂ arena, these analyses support the program's high level goals of developing technologies to ensure 99% storage permanence by providing tools for the detection of CO₂ migration from the target sequestration reservoir. In the arena of unconventional resources, these analyses provide a suite of naturally-occurring geochemical tracer tools that can help verify the sources of fluids in complex geologic systems.



Analytical chemist working with the inductively coupled plasma mass spectrometer.

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Capabilities

Conventional analytical techniques currently used at NETL include the measurement of bulk parameters including pH, alkalinity, conductivity, dissolved oxygen, and oxidation-reduction potential as well as constituent-specific measurements of cations and anions. The suite of analytical instruments includes inductively coupled plasma optical emission spectroscopy (ICPOES), inductively coupled plasma mass spectrometry (ICP-MS), ion chromatography (IC), and cold vapor atomic fluorescence (CVAF), which is specific for mercury. Conventional analyses are done using standard analytical techniques (e.g., EPA-established techniques).

In addition to the routine conventional techniques, cutting edge instruments are being used to probe the complex chemistry that can occur among water, CO₂, and geologic media in the sub-surface. Isotopic measurements are performed using isotope ratio mass spectrometry (IRMS), and multi-collector inductively coupled plasma mass spectrometry (MC-ICPMS). The isotope facilities housed at the University of Pittsburgh Department of Geology and Planetary Sciences clean laboratory facility and the Stable Isotope Facility at the Geology Department of West Virginia University are considered in more detail in a separate Fact Sheet.

Other research methods include:

- High-pressure liquid chromatography–inductively coupled mass spectrometry (HPLC-ICPMS) for element speciation.
- Liquid chromatography quadrupole time of flight mass spectrometer (LC-QTOF) for the analysis of liquid-phase organic compounds. This instrumentation provides various ionization modes depending on the organic class of interest. Secondary detection options include photodiode array, ultraviolet/visible, and fluorescence absorption.
- Analytical research grade IC for matrix-sensitive or redox-sensitive anions.
- CO₂ coulometer and portable CO₂ analyzer for the direct analysis of dissolved CO₂ concentrations in aqueous samples.
- Electrochemistry techniques for analysis of trace elements and oxidation-reduction processes using micro-redox probes and voltammetry.
- Microbiological analyses are discussed in a separate Fact Sheet.

Benefits

These techniques are of direct relevance to NETL research areas, including the monitoring, verification, and accounting program; multi-scale, multi-phase fluid flow; chemistry of co-produced waters, brines, and hydraulic fracturing fluids; interaction of aquifers and production waters with geologic media such as confining layers and fossil fuels (e.g., coal, oil shale, natural gas bearing formations); and unconventional fossil fuel extraction techniques.

The use of geochemical analyses provides geochemical information complimentary to that obtained using geophysical methods, and both are integrated in NETL program areas. The use of naturally occurring major, minor, and trace elements as indicators of sub-surface activity provides an understanding at the mineral and chemical levels of the larger processes at work in geologic settings.



NETL's Multicollector ICP MS instrument, currently housed at the University of Pittsburgh, is used to measure isotope ratios in natural samples.

Accomplishments

A number of NETL's fluid chemistry analytical techniques, including ICP-OES and strontium isotope ratio analysis, were recently applied to an examination of the sub-surface hydrology and geochemistry at a natural analog site in Chimayó, NM. In this work, which was a collaborative effort with participants from NETL, the University of Pittsburgh, and Los Alamos National Lab, the water quality observed in wells in the area could be explained in some cases by a mixing between CO₂-rich brine and low-total dissolved solids (TDS) waters, but CO₂-induced dissolution of aquifer carbonate was most likely occurring in others. Such information assists in the understanding of complex sub-surface interactions that can occur when CO₂ comes in contact with geologic media and is important for understanding the possible effects of geologic CO₂ storage. ("Tracking CO₂ migration through a sandstone aquifer using Sr isotopes: Chimayo, New Mexico, USA," presented during the Goldschmidt Conference, Knoxville, 2010).