This Week at NETL

January 13, 2014

Site-Characterization Project in Southwestern Wyoming Completed

The University of Wyoming Carbon Management Institute (CMI) has concluded its NETL-sponsored site-characterization project evaluating the potential of a geologic formation called the Rock Springs Uplift to provide long-term, high-volume storage for carbon dioxide (CO_2) produced by coal-fired power plants and other large anthropogenic sources. A wealth of geologic, hydrologic, and geochemical data were gathered from a 12,810-foot-deep stratigraphic test well drilled into the formation in southwestern Wyoming. The project team collected, photographed, and analyzed more than 900 feet of whole core, and obtained a comprehensive wireline (cable) log suite from the test well. Fluid samples from the targeted storage zones suggest that reservoir brines contain high concentrations of lithium, which could be processed to generate revenue to offset the cost of a future CO_2 storage operation. Digital geophones were used to create a microseismic baseline at the site, which will enable the future identification of induced micro-fracturing related to CO_2 injection. In addition to the characterization well, project researchers have completed a 5-mile by 5-mile, three-dimensional seismic survey around the well site. The key storage formations within the Rock Springs Uplift are the Weber-Tensleep Sandstone and the Madison Limestone, at depths of approximately 11,500 feet and 12,500 feet, respectively. It was demonstrated that the overlying Dinwoody formation, at a depth of 10,600–10,800 feet, is a world-class confining zone that traps helium and will contain the stored CO_2. Realistic estimates suggest that the targeted formations could store 14–17 billion tons of CO_2, representing 250–300 years' worth of the CO_2 emissions in the state. CMI has submitted the draft final report for the project, which concluded December 7, 2013.

Early Testing Demonstrates Potential of New Sensor Material

Preliminary results of an NETL-sponsored project at the University of Texas at El Paso show that a tungsten-doped gallium oxide nanostructured material may make an excellent oxygen sensor for use in advanced energy systems where high temperatures and harsh environments limit the use of more conventional sensor materials. During the most recent quarter, the optical response of tungsten-doped gallium oxide films was tested under controlled conditions, specifically in the presence of hydrogen and oxygen at a temperature of 600 degrees Celsius. The optical response of the films demonstrated repeatability, and increasing wavelength resulted in a stronger response. Incorporation of hydrogen generated an increasing response on the absorption spectra, whereas oxygen-rich gas (air) produced a decrement in the absorption curve. No deterioration was noted over time. Complete results can be found in the project's latest quarterly report.

Computational Tool Constructed To Examine Transport Properties in Nickel-Based Alloys

NETL researchers have constructed a computational tool to examine transport properties in nickel-based alloys. The tool is based on Kinetic Monte Carlo framework, which allows modeling of atomic jumps at laboratory conditions. A computationally efficient analytical expression captures the effect of the local environment, and the *ab initio* "trained" model expression permits determination of hopping barriers under different local environments. This is otherwise impractical to calculate from *ab initio* methods alone, even with the most efficient computer hardware. The entire computational machinery was implemented in an in-house software code. An earlier version of the tool is described along with its application to the nickel-plus-oxygen system in a manuscript titled "First-Principles Studies on Vacancy-Modified Interstitial Diffusion Mechanism of Oxygen in Nickel, Associated with Large-Scale Atomic Simulation Techniques." The manuscript has been accepted for publication in the *Journal of Applied Physics*.

Manuscript Accepted for Publication in Spectroscopy Journal

As part of laser-induced breakdown spectroscopy (LIBS) down-hole sensor research, NETL investigated how the concentration of sodium can have a significant effect on the measurement of other atomic species in water samples. The work is reported in a peer-reviewed manuscript titled "Effect of Sodium Chloride Concentration on Elemental Analysis of Brines by Laser-Induced Breakdown Spectroscopy (LIBS)," which has been accepted for publication in the February 2014 issue of *Applied Spectroscopy*. The ultimate goal of LIBS is the development of a rugged, miniaturized laser sensor system that can report real-time atomic and molecular concentrations from the down-hole environment.

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