netlog

NETL's R&D newsletter

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Laser Spark Plug Overcomes Barrier

Two Technology Transfer Awards

New Probe for Pipeline Integrity

CONTENTS

ON THE COVER

NETL scientist Steven Woodruff is evaluating a photonic crystal optical fiber as a Raman sensor for gaseous materials.

netlog is a quarterly newsletter which highlights recent achievements and ongoing in-house research at NETL. Any comments or suggestions, please contact Paula Turner at paula.turner@netl.doe.gov or call 541-967-5966.

NETL's Laser Spark Plug Overcomes Barrier to Operate Smoothly

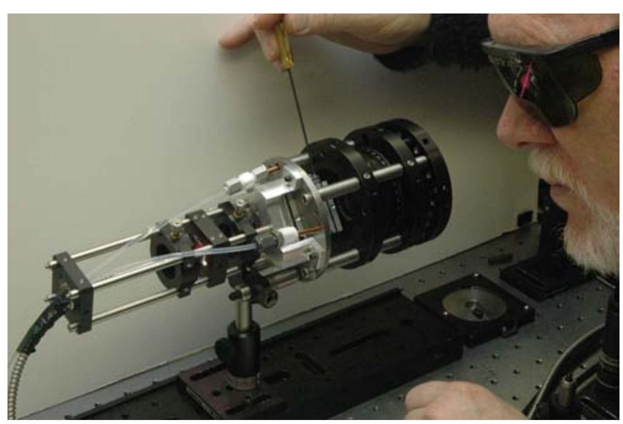
A laser spark plug developed at NETL has overcome one of the barriers to laser distribution through optical fibers. Testing has been completed of an end-pumped laser spark plug on a single-cylinder research engine. The engine was operated on natural gas and also on natural gas augmented by 20 percent volume hydrogen.

In three days of testing, the engine operated smoothly through a range of conditions with multiple startups and shutdowns. The laser ignition approach can permit engine operation at higher efficiency and with reduced emissions.

A barrier to laser distribution with optical fibers has been the high laser power required to initiate a laser spark. The spark plug developed by NETL overcomes that barrier in a unique way by utilizing a compact Q-switched laser located at the engine cylinder, which is pumped by a diode laser from one end through an optical fiber. In this configuration, the laser power delivered is low enough to avoid damage to the fiber.

NETL is working with a CRADA partner to improve packaging and performance of the Q-switched laser and is seeking another CRADA partner to help develop its patented pump energy distribution system.

Contact: Steve Woodruff, 304-285-4175



Dr. Steven Woodruff adjusts the NETL laser spark plug to prepare it for installation on the Ricardo single-cylinder, large-bore engine for testing.

Representatives of some of the institutions collaborating on the research examine a flow cell. They include Duane H. Smith, seated, an NETL Geosciences Division Senior Scientist and Adjunct Professor in the Department of Physics at West Virginia University; Dustin Crandall, standing left, a National Research Council Associate at NETL; and Goodarz Ahmadi, Dean of Engineering at Clarkson University.

NETL Leads International Team on CO_2 Brinefield Storage

Researchers at NETL are leading an international team of collaborators on important research related to geological storage of carbon dioxide and increased oil production. NETL, West Virginia University of Morgantown, WV, and Clarkson University of Potsdam, NY, have been working together on a program of laboratory experiments, computations, and theory to develop more accurate and reliable equations for describing multiphase flow through porous media. The University of Utrecht in the Netherlands recently joined this effort and is working with scientists and engineers at the other three institutions.

Important applications include injection of water into oilfields to increase the production of petroleum and injection of carbon dioxide into brine-saturated geologic strata to reduce atmospheric concentrations of carbon dioxide and global warming.

In the first stage of this new collaboration, experiments performed at NETL will provide values of parameters to use in a thermodynamic model of two-phase flow through porous media. The equations for the thermodynamic model had been previously developed in separate work at Utrecht and by the NETL-Clarkson-WVU group.

Contact: Duane Smith, 304-285-4069

Barbara Kutchko uses a series of high-pressure vessels manufactured specifically for NETL's Geologic Sequestration Core Flow Laboratory, currently used in evaluating the potential for cement degradation to affect storage integrity for geologic storage of carbon dioxide.

Research Suggests Cement Plugs Will Resist Degradation by CO_2

Research conducted at NETL shows that imperfections (air pockets, cracks, etc.) in cement can lead to significant risk to storage integrity, but chemical degradation of cement is unlikely to be extensive enough to present a significant risk to storage integrity of CO_2 under geologic sequestration scenarios. The results were in excellent agreement with field samples from an enhanced oil recovery site exposed to CO_2 for 30 years. Both the nature and extent of reaction were as predicted by NETL's laboratory experiments. NETL researcher Barbara Kutchko presented these findings at an invited seminar at Princeton University.

The cement used to install and/or plug existing wells is critical in preventing leakage of CO_2 to the surface under geologic sequestration scenarios. NETL has conducted laboratory experiments to determine the risk of storage loss due to chemical reaction between CO_2 and cement. The recent experiment was one year in duration. Results were extrapolated to predict longer-term behavior.

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NETL Receives Two National Technology Transfer Awards

The Federal Laboratory Consortium (FLC) will present national technology transfer awards to NETL for two innovative technology transfer successes at its national conference in Portland, OR, on May 8. The Award for Excellence in Technology Transfer recognizes laboratory employees who have accomplished outstanding work in the process of transferring a technology developed by a federal laboratory. Nominations are made by FLC laboratory representatives and are judged by representatives from industry, state and local government, academia, and federal laboratories.

The FLC 2008 Award will be presented for technology transfer that resulted in a license to Johnson Matthey for commercial development and application of NETL-invented palladium-based sorbents for high temperature capture of mercury, arsenic, and selenium from fuel gas. Gasification is an important strategy for increasing the utilization of abundant domestic coal reserves in an environmentally friendly manner. High temperature capture of the trace elements mercury, arsenic, and selenium helps preserve the high thermal efficiency of integrated gasification combined cycle (IGCC) plants versus low temperature capture by activated carbons. The sorbents are described in U.S. Patent 7,033,419, issued in April 2006 and in recent publications in the journals *Industry and Chemistry Research* and in *Fuel.*

The second award is for transferring NETL's Coal Chemistry Module to Fluent as well as to KBR and Southern through its applications. NETL researchers are using the coal chemistry module with both MFIX (Multiphase Flow with Interphase eXchanges) and the commercial code Fluent to model different coal gasification processes. The Coal Chemistry Module software, developed at NETL, incorporates detailed reaction mechanisms for devolitization, tar cracking, moisture release, gasification, and combustion for different bituminous, subbituminous and lignite coals into Eulerian-Eulerian Computational Fluid Dynamics (CFD) models. This unique capability allows investigation of coal reactivity, while simultaneously accounting for the surrounding hydrodynamic conditions predicted by a Eulerian-Eulerian CFD model.

Jeff Culp, a researcher at NETL, examines a sample of carbon dioxide adsorbents composed of layers and pillars, which may find applications in such technologies as gas purification, gas storage, and sensors.

NETL Conducts Systematic Study of Carbon Dioxide Adsorbents

In the continuing search for better adsorbents for carbon dioxide, the relationship between performance and molecular structure becomes a key guiding principle.

NETL researchers have conducted a complete study of the relationship between performance and molecular structure of a series of carbon dioxide adsorbents composed of layers and pillars.

The layers consist of sheet-like nickel cyanide complexes. They are held apart by organic pillars of different length and flexibility. Carbon dioxide storage capacity was related to the relative size of the pores and greater capacity was associated with pillars of greater length. The adsorption strength was strongly affected by whether the pillars were rigid or flexible. The adsorbent made with the most flexible pillar had a collapsed pore structure that was ineffective in adsorbing carbon dioxide while those made with rigid pillars had open pores that readily took in carbon dioxide.

The pillared layered architecture has been found to be an excellent scaffold on which to study the effect of molecular structure on adsorbent behavior. This technique is now being extended by investigating the effect of attaching organic functional groups with stronger affinity for carbon dioxide to the pillars.

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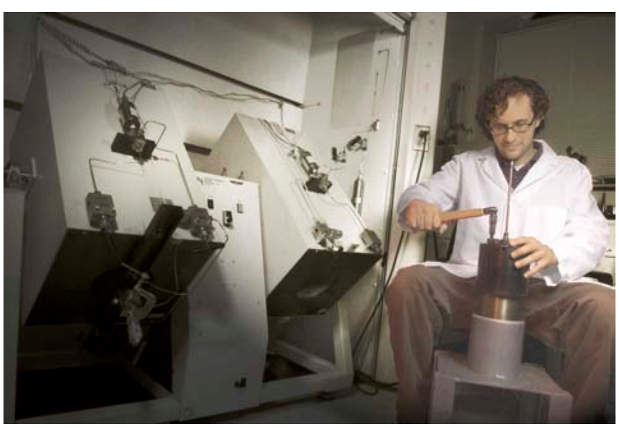

Robert Dilmore, a researcher at NETL, assembles a pressure vessel reactor to place in the hydrothermal rocking autoclave. Dilmore is part of a team of scientists investigating carbon dioxide/water/rock interaction for CO_2 storage in deep saline aquifers and other geological formations.

NETL Researchers Develop Method to Estimate CO_2 Storage Capacity in Oriskany Formation

As part of NETL's ongoing research into geologic sequestration of anthropogenic CO_2, results of an investigation into solubility capacity of the Oriskany Sandstone brine aquifer in the Appalachian Basin will appear in an upcoming special edition of the ACS journal *Environmental Science and Technology*. Rocking autoclave reactors were used to measure the solubility of CO_2 in real brines of the Oriskany formation at in-situ conditions, and these data were used to validate a model developed by Duan and Sun.

Using available geospatial data, this empirically verified model was applied within a geographic information system to develop an estimate of the solubility capacity of CO_2 in the Oriskany formation: 0.36 gigatons of CO_2. This estimate provides a low-boundary of formation capacity, as compared to a volumetric (free-phase) supercritical CO_2 capacity estimated to be approximately 8.8 gigatons.

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U.S. Army Seeks NETL's Help During Cast Steel Armor Meeting

NETL scientist Paul Turner explained P900 armor and described various methods to manufacture the material at a meeting on March 19 to identify potential manufacturers of cast steel armor for the Department of Defense. NETL scientists, working under a contract from DoD, developed the process to make P-900, which is a cast, slotted steel armor. The purpose of the meeting was to expand the current number of foundries manufacturing the armor to meet the military's large demand for the material in a short timeframe. During the meeting, Army representatives requested NETL's help to develop a new, lighter weight ferrous alloy for use in this application. The U.S. Army hosted the manufacturing meeting in conjunction with Missouri University of Science and Technology and the Steel Founders' Society of America. The U.S. Army Tank and Automotive Command (TACOM) is in the process of procuring over 20 million pounds of P-900 cast steel armor to be used on certain U.S. military vehicles to protect them from improvised explosive devices, which have been very effective against coalition vehicles. Approximately 80 representatives of the foundry industry, DoD agencies, academia, and vehicle manufacturers attended the meeting.

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NETL Helps Siemens Model Advanced Gas Turbine Concept

NETL is assisting Siemens in developing computational fluid dynamics (CFD) modeling efforts of the Low Swirl Injector (LSI). NETL researcher Dr. Peter Strakey attended a meeting at Siemens, Orlando, to discuss the effort. Siemens has been developing the LSI, patented by Dr. Robert Cheng of Lawrence Berkeley National Laboratory, as a novel piloting technique for its current line of natural gas-fired turbine combustors. NETL has been working with Dr. Cheng over the past year by conducting tests on the LSI in NETL's SimVal combustor with both natural gas and hydrogen fuels. CFD modeling and validation of the LSI has been conducted at NETL as well as an effort to develop and validate Large Eddy Simulation (LES) tools for gas turbine combustor modeling. Siemens has been attempting to use a commercial CFD code (CFX) to model the flow field produced by the LSI, but with little success. The company's modeling efforts are geared toward optimizing the integration of the LSI into the combustor for piloting purposes. The meeting, which was attended by Dr. Cheng as well as several other groups (Georgia Tech and Stanford), was an effort to discuss various modeling approaches and aid Siemens in its modeling efforts. Siemens also expressed interest in obtaining the experimental data on the LSI collected at NETL. The data, which has already been sent to Siemens, will aid in validation of the company's CFD modeling approaches.

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New Probe Developed for Plastic Natural Gas Pipeline Integrity

Dr. Mahendra Mathur of NETL and REM Engineering researchers working at NETL published their work on in-situ detection of defects in buried plastic natural gas pipeline in the American Institute of Physics' peer-reviewed journal *Review of Scientific Instruments*. The paper describes a probe developed by NETL to determine the in-situ integrity of plastic natural gas pipeline from the interior. The probe has its own internal power source and can be deployed into existing natural gas pipelines. A proprietary electronic circuit design allows for data to be transmitted in real time or stored on board for later evaluation.

The circuit will theoretically allow the detection of voids 1/4-inch long, 1/40-wide, and 1/40- inch deep. This resolution should allow the detection of brittle cracks developed due to aging of pipes. Utilizing the capacitance parameter, the probe inspects the pipe for flaws and internally records the data, which can be retrieved later for analysis. Since the decade of the 1970s, many of the newly installed gas distribution and transmission lines in the United States are fabricated from polyethylene plastic. Reliability of the natural gas transmission and distribution network across the United States is essential to ensure the availability of clean, affordable energy to our homes, businesses, and industries. The development of technology to ensure a continued high level of integrity and reliability is necessary. In the post 9/11 era, safeguarding our infrastructure against terrorism has become crucial. To that end, a device to monitor the integrity of the plastic gas pipelines has assumed much importance. Several techniques are available to determine the integrity of in-situ metal pipelines but very little is available in the literature to determine integrity of plastic pipelines.

The paper appeared in the journal's December 18 issue.

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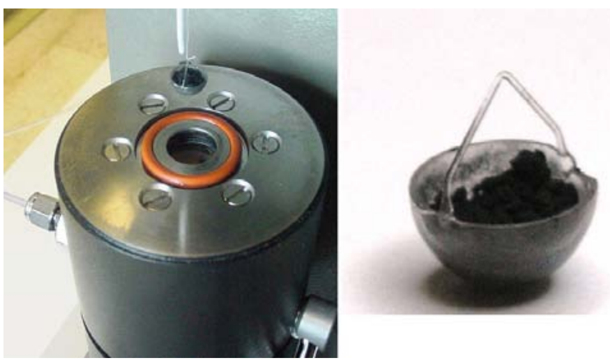

The coal-metal oxide sample in the Thermogravimetric analysis unit.

Chemical-Looping Combustion Research Shows Promising Results

Challenges that have prevented chemical-looping combustion (CLC) from becoming an economical way to combust coal need to be dealt with, and NETL researchers are currently addressing these challenges.

Chemical looping has been proposed as a method to conduct combustion with inherent CO_2 separation. The separate CO_2 stream could then be sent to geologic storage without the complexity of scrubbing flue gas to capture CO_2. In chemical-looping systems, carbon-containing fuels can be oxidized with a metal oxide that provides the oxygen for consuming the fuel. Similar to oxy-fuel combustion, the products are just CO_2 and water (plus the reduced metal). Unlike oxy-fuel combustion, no oxygen supply is needed. Instead, the reduced metal can be re-oxidized with air in a separate reactor and recycled back to the fuel reactor, thus the name "chemical looping." This idea has already been demonstrated for gas fuel combustion. Less attention has been given to solid fuels, probably because of the perceived difficulty of reacting the solid fuel with the metal oxide without a significant gas-phase mediator between the solid phases.

Results of laboratory-scale tests at NETL strongly support the feasibility of utilizing metal oxide oxygen carriers as a method of transferring oxygen from air for coal combustion that would involve no other air constituents. Samples of coal mixed with oxides of copper, nickel, and manganese were heated in the presence of CO_2. Coal-combustion was observed at 600-800 ºC. The reduced metals were re-oxidized to recover the metal oxide, completing the chemical-looping cycle. Direct combustion of coal utilizing metal oxide oxygen carriers showed full combustion of coal in the presence of CO_2.

If the NETL research overcomes the challenges, CLC could become a very economical way to utilize coal.

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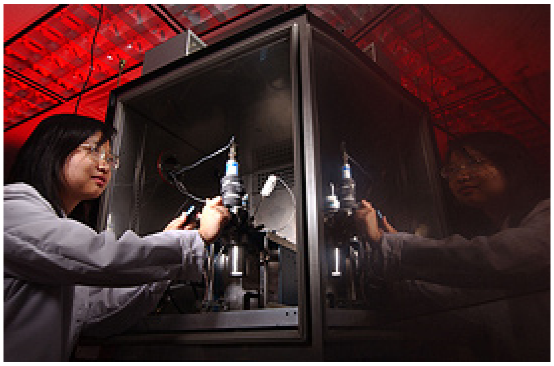

Yi Zhang, a research associate in the Geosciences Division, prepares an experiment in one of the high-pressure reactors associated with NETL's Hydrate Facility.

Research Adds To Knowledge of Hydrates

Research key to understanding the formation and stability of hydrates in nature and the impacts of these processes in engineered scenarios was published in an article in *Industrial & Engineering Chemistry Research* in January 2008. Hydrates are seen as a possible source of great amounts of natural gas. This work is relevant to modeling the phase behavior of hydrate, which is important in determining the formation and dissociation of methane hydrate in production, climate change, and seafloor stability scenarios and carbon dioxide hydrate in sequestration scenarios when contact is possible with cold, water-containing systems.

Experimental work was performed with carbon dioxide; and theoretical predictions were made for this gas and for methane using a modified thermodynamic model.

The title of the manuscript is "Phase Equilibrium in Two-Phase, Water-Rich-Liquid, Hydrate Systems: Experiment and Theory." It was coauthored by Dr. Yi Zhang, who received her doctorate degree at the University of Pittsburgh based on this work, which was performed at NETL; Dr. Gerald Holder, US Steel Dean of Engineering at the University of Pittsburgh, who was her research advisor; and Robert P. Warzinski, her mentor at NETL. The paper describes the formation of hydrate from a hydrate-forming gas dissolved in aqueous solution in the absence of any separate gas or liquid phase of the hydrate former.

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