# netlog

NETL's R&D newsletter

Issue 8, January 2008

## Hydrates Across the Globe

## Water Management Model

## New Laser Spark Plug

U.S. Department of Energy • Office of Fossil Energy • National Energy Technology Laboratory

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## ON THE COVER

Kelly Rose, of NETL's Office of Research and Development, aboard the drillship *Rem Etive*.


*netlog* is a quarterly newletter 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 Researchers Pursue Gas Hydrates Across the Globe

Over the past 18 months, NETL researchers have pursued natural gas hydrates from the Equator to the Arctic Circle, including several different cooperative expeditions in the Bay of Bengal, Andaman Sea, East Sea/Sea of Japan, South China Sea, Gulf of Mexico, and Alaska North Slope. Gas hydrates are solid combinations of natural gas and water that are found in environments of high pressure and/or extremely low temperatures such as the Arctic regions and within shallow sediments of deep-water continental shelves across the globe. They have immense potential as a future energy resource and are also an important, yet poorly understood, component of the global carbon cycle and global climate change.

*Kelly Rose examines sediment cores from the Indian Ocean.*

Earlier this year, Kelly Rose helped forge new international collaborations for DOE by participating as a geologist and sedimentologist for separate

one-month expeditions in the South China Sea and South Korea's East Sea. Rose participated in these two separate international gas hydrate expeditions at the invitation of Geotek, a marine service company commissioned to conduct shipboard research activities during these studies.

In May 2007 Rose participated in China's four-week drilling and coring expedition in the South China Sea; and in October 2007 Rose served as lead sedimentologist for South Korea's 5-week methane hydrates coring and drilling expedition in the East Sea. The goal of both the Chinese and South Korean efforts was to test pre-expedition exploration techniques for identifying the location and occurrence of sub-seafloor methane hydrate accumulations and fully characterize those accumulations through drilling and coring activities and subsequent analyses.

In addition, in July 2007 Rose and NETL's Eilis Rosenbaum participated in the Naval Research Laboratory's two week expedition in the deepwater Gulf of Mexico's Aliminos Canyon region. This study collected shallow sub-seafloor piston cores and thermal gradient data to help constrain models for fluid and methane flux in the region. NETL scientists will continue to make critical contributions to projects that advance the understanding of the geological controls, occurrence, and physical behavior of gas hydrates in nature through a variety of efforts including geological characterization, numerical simulation, and laboratory based studies. For complete story, click here.

Contact: Ray Boswell, 304-285-4541

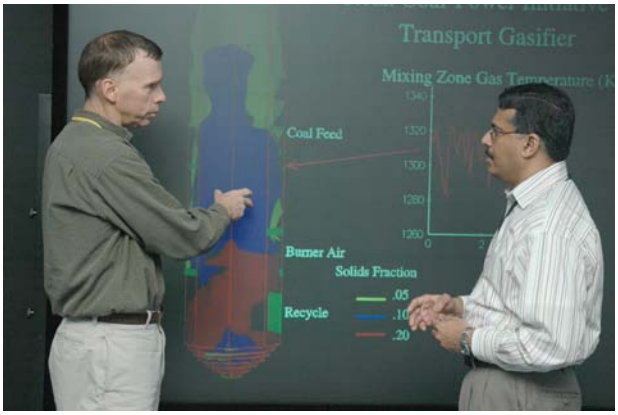
*An example of a coalbed natural gas infiltration impoundment.*

### Industry Requests NETL-developed Water Management Model

Attracted by an article titled *Improving Water Management* in the January-March issue of ArcUser magazine, world leading independent oil and gas explorer-producer Devon Energy plans to evaluate a NETL-developed computer model that screens candidate impoundment locations for minimum environmental risk associated with storing or disposing produced water from natural gas. Developed in cooperation with the University of Pittsburgh with Modelbuilder software available from Environmental Systems Research Institute (Redlands, CA), the GIS-based decision-support model incorporates digital elevation data and helicopter electromagnetic geophysical results to screen potential sites for coalbed natural gas-produced water-disposal impoundments. The goal is to identify sites for impoundments with maximum soil absorption.

This computer model could also be used to screen for other types of potential site locations.

Contact: Jim Sams, 412-386-5767




*Chris Guenther, left, and Madhava Syamlal discuss the results of a transport gasifier simulation produced by MFIX.*

## NETL Launches High-Resolution Simulation of Commercial-Scale Transport Reactor

NETL's Computational Science Division's Multiphase Flow Research Group is taking advantage of supercomputer time allocated by the DOE Undersecretary for Science, using MFIX (Multiphase Flow with Interphase eXchanges) code to investigate the performance of a transport gasifier at Orlando, FLA. The gasifier is part of a Clean Coal Power Initiative project managed by NETL.

Results from these high-resolution simulations will be used to verify earlier simulation results and will be shared with industrial stakeholders using this information in the design of their commercial-scale transport gasifiers.

The Undersecretary, Dr. Ray Orbach, allocated 500,000 hours of computer time on the CRAY XT4 system at the National Center for Computational Science to NETL to increase the speed of MFIX using massively parallel computations and to enable high-resolution gasifier simulations. Previous simulations found that the coal injection velocity and syngas recycle rate has a significant effect on the peak temperature and that these temperatures can exceed the recommended maximum operating temperature of the refactory-lined walls.

The previous simulations were conducted on computer clusters at NETL and at the Pittsburgh Supercomputing Center. Typical simulations required approximately 2 million computational cells and were run in parallel using 20 to 40 processors. The more recent work resulted in factor-of-3 improvements in the parallel efficiency of MFIX and allowed gasifier simulations to be conducted using 10 million computational cells running on 2,048 processors. This is a 50-fold increase in the number of processors used over previous simulations.

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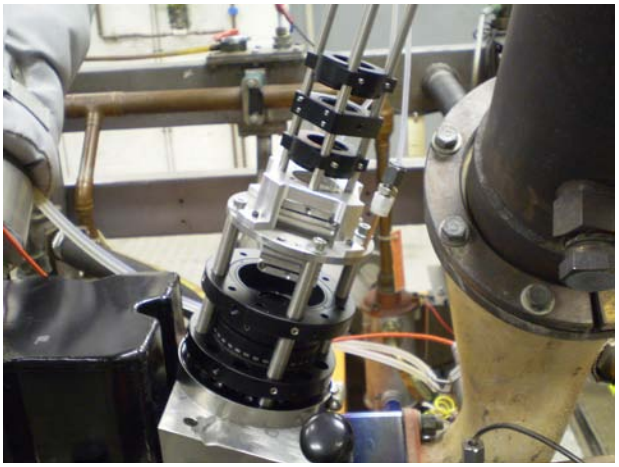

*The laser spark plug is mounted on the single cylinder Ricardo Proteus engine in the NETL engine lab. The aluminum colored block in the middle is the laser with the optical fiber pump optics above it. Immediately below is a beam steering apparatus which directs the laser pulse to a lens window where an electric spark plug's electrodes would normally be. The lens window focuses the laser pulse to form a plasma spot in the cylinder.*

## New Laser Spark Plug Improves Function of Test Engine

The NETL single-cylinder research engine was started and run on natural gas fuel using an end-pumped laser spark plug developed by NETL research staff. The laser spark plug designed and built at NETL is an end-pumped, passively Q-switched, Nd:YAG laser with the pump light delivered by fiber optic. In March of 2007, NETL researchers demonstrated a prototype laser spark plug using a miniaturized diode-pumped solid-state laser. Those tests proved the concept but engine

vibrations impacted laser performance. The new spark plug provides a more rugged design and uses a fiber optic delivery system to pump the laser. It also provides more consistent spark delivery enabling the engine to be started cold and run continuously for longer periods. The compact design produces a 6-9 millijoule laser pulse 2.5 nanoseconds long, which generates a spark through an NETL-designed lens. The lens is mounted in a spark plug housing and provides the pressure seal as well as focusing the plasma spark 6 mm inside the cylinder. The engine was initially test fired on the laser plug on December 5 for ~15 minutes. During that time, the engine was run at up to 1,800 rpm, the target testing speed. A full-test plan to evaluate engine and laser spark performance was performed the following week involving operating the engine with laser spark approximately 8 hours over three days of testing. The laser spark plug was tested on natural gas and hydrogen augmented natural gas, a mixture of 80 per cent natural gas and 20 per cent hydrogen by volume over a range of air-fuel ratios.

Contact: Steven Woodruff, 304-285-4175


*Researchers prepare NETL's Ricardo Proteus engine for hydrogen-fueled test operation.*

### Researchers Complete Tests of Lubricating Oil Formulation on Emissions From Hydrogen-Fueled Reciprocating Engines

This work is part of NETL's University Research Initiative and involves the collaboration of NETL, West Virginia University, and the National Institute for Occupational Safety and Health (NIOSH) laboratory located in Morgantown, WV. Researchers from NETL and West Virginia University recently completed experiments designed to investigate the effects of different lubricating oil formulations on the oil consumption and mutagenicity of particulate emissions from hydrogen-fueled reciprocating engines.

The collected data will be useful in improving and assessing improved lubricating oil formulations for hydrogen-fueled reciprocating engines.

Earlier work at NETL and by other investigators suggests that a significant portion of the mutagenic particulate emissions from reciprocating engines arises from the lubricating oil. These findings are confounded, however, by the difficulty in separating emissions originating from the fuel from those originating from the lube oil.

The recently completed engine tests were conducted using hydrogen as the fuel so that all particulate emissions could be ascribed to the lube oil. Particulate samples collected during the recent engines tests have been delivered to NIOSH for mutagenicity testing, which is expected to take several weeks.

Early results show accelerated lubricating oil deterioration in hydrogen-fueled engines compared to other fuels. Data collected on engine performance, emissions, and oil consumption are now being analyzed. When data analysis is complete, the effects of lubricating oil formulation and engine operating parameters on emissions will be quantified and submitted to a peer-reviewed journal for publication.

Contact: John Ontko, 304-285-4930

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*Jeff Culp examines a sample of a dynamic metal organic framework material that may find applications in such technologies as gas purification, gas storage, and sensors.*

### New Applications Explored for Unusual Carbon Dioxide Adsorbent

NETL scientists have created a new adsorbent for carbon dioxide that shows very unusual behavior. They are exploring possible applications of this unusual adsorption behavior in the areas of gas separation, gas purification, and in-gas sensing devices.

The adsorbent is a flexible, pillared-layer compound. It is one of a new class of materials called metal organic framework or MOF. The layers are sheets of an ionic nickel complex and the pillars are a specially selected organic compound. Once the sheets and pillars are interlayered to form galleries of open channels, gas molecules may be inserted into them.

In the absence of carbon dioxide, the pillars are tilted and the structure is partially collapsed. As carbon dioxide is adsorbed into this structure, the pillars lose their tilt and the structure opens to accommodate more gas molecules.

Most adsorbents used to capture gases have rigid structures that fill with increasing pressure and empty with decreasing pressure in a reversible way. When the new adsorbent is being filled with carbon dioxide, a certain threshold pressure of carbon dioxide is required to force the structure open. Once the structure is full, the pressure is released, but the opened structure retains carbon dioxide until a very low pressure is reached. As the carbon dioxide exits, the adsorbent returns to its previous collapsed structure. The flexible nature of this structure depends on the exact structure of the pillar.

The achievement of this degree of control over the properties of a family of porous materials marks a real advance in adsorption science. A manuscript is being prepared for publication describing the results of this study.

Contact: Bradley Bockrath, 412-386-6081

*Researchers Granite (left) and Pennline invented technology to detect mercury in flue gases.*

### Researchers Invent Mercury Detection Technology

NETL inventors Evan Granite and Henry Pennline have added a mercury detection technology to their portfolio of several mercury removal technologies. Their new invention detects mercury in flue gases, which will make it possible for power plant operators to verify compliance with regulations either issued or pending at the Federal level and in 26 states.

The patent-pending detection technology can be used with any mercury removal technology to determine how much mercury is present before coal is burned and how much remains after combustion. The technology is a spin-off of the GP-254 removal technique, which irradiates flue gas with ultraviolet light.

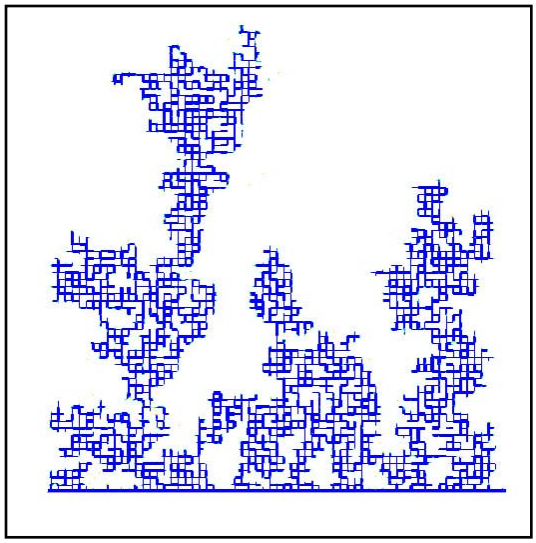
Pennline and Granite previously patented three mercury control technologies that have been licensed to industry for commercial use in removing mercury from coal-derived flue gases, including the GP-254 technique. The new technique works by blending a small slipstream of hot flue gas with oxygen or air, and subsequently irradiating it with ultraviolet light having a wavelength of 254-nanometers. Measuring the mercury in the resulting deposited mercuric oxide allows for the rapid determination of mercury concentration in the flue gas.

The United States Environmental Protection Agency recently issued a regulation for the reduction of mercury emissions from coal-burning utilities. Twenty-six states have legislation or pending legislation for mercury control on coal-fired power plants.

Mercury is present within coal-derived flue gases at infinitesimally small concentrations. The typical concentration of mercury in untreated coal-derived flue gas is on the order of one part-per-billion while treated flue gases often have sub part-per-billion mercury levels.

The mercury in flue gas exists as elemental, oxidized, and particulate bound forms. The extraordinarily small concentrations, different mercury species, and the numerous reactive moieties present within flue gas complicate the determination of mercury.

Contact: Evan Granite, 412-386-4607

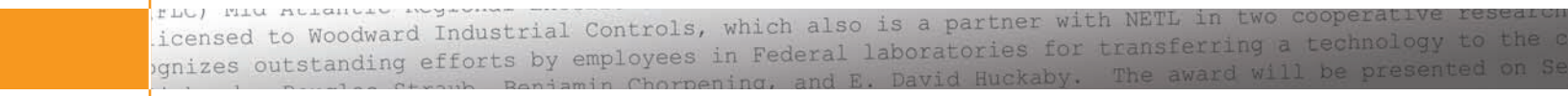


*Numerical Saturation Profile. Air into Water.*

### Method Developed to Improve Sequestering Carbon Dioxide in Brine Fields

NETL researchers have developed a new method to design and fabricate flow cells for laboratory studies to improve carbon dioxide sequestration in brine fields. This new method uses stereolithography (SL) to fabricate the cells. During production, a laser cures a thin layer of photo-sensitive resin on the surface of a vat of liquid resin; a moveable platform then submerges the cured layer and a new layer is cured on top of the previous one, creating a physical model from a computer-generated model. This layered fabrication of a computer-generated model has enabled the production of an experimental porous medium with improved fluid resistance properties, as compared to previously studied etched cells. This work was presented at the American Geophysical Union Fall Meeting, San Francisco, December 10-14, 2007. A paper describing this work has been submitted to the peer-reviewed journal Experiments in Fluids.

Contact: Duane H. Smith, 304- 285-4069




## Licenses

### NETL Licenses Emissions-Capture Invention to Jupiter Oxygen Corporation

NETL has licensed an emissions-capture invention to Jupiter Oxygen Corporation. Invented by Jupiter Oxygen and federal researchers at NETL, the patented technology was developed under a Cooperative Research and Development Agreement. The invention provides a means for removing pollutants from new and existing power plant flue gas at lower overall cost with greater fuel efficiency and delivering a stream of $CO_2$ alone or with other waste elements. The result is capture of the entire combustion vapor/gas stream for sequestration and a near-zero emissions power plant. This invention combines Jupiter Oxygen's oxy-fuel combustion expertise with NETL's expertise in $CO_2$ purification and compression and energy recovery.

Contact: Cathy Summers, 541-967-5844

### Method to Capture Acid Gases and $CO_2$ From Flue Gas Licensed to Powerspan

A technique invented at NETL to capture acid gases and $CO_2$ from flue gas at coal-burning power generation point sources has been licensed to Powerspan Corp. of New Durham, NH. This regenerable absorption process uses an ammonia-based solution to remove $CO_2$ and acid gases, primarily $SO_2$ and $NO_x$. Fertilizer, a salable commodity, is produced in the process and the spent ammonia solution is regenerated and recycled back to the scrubbing unit. The licensed patent will expand Powerspan's efforts to remove all components from flue gas. Powerspan has committed to constructing a 1-MW scale demonstration of the licensed technology at First Energy's Berger Station in Shadyside, Ohio.

This technology has the potential for significant reduction in capital cost and energy load for $CO_2$ capture as compared to existing technology. The advent of the carbon sequestration area within DOE's Fossil Energy program prompted the investigation of various techniques to capture $CO_2$ from coal-burning power generation point sources. One technique developed by NETL to capture carbon dioxide from flue gas uses an aqueous ammonia-based scrubbing solution. Under a cooperative venture in the form of a CRADA, Powerspan and NETL collaborated to understand an ammonia-based, regenerable wet scrubbing process that removes all acid gases and trace components, for example mercury, from the flue gas. Powerspan Corp. had developed its ECO process that uses ammonia solution to scrub the acid gases, excluding $CO_2$, from the flue gas to produce a fertilizer and to reduce mercury emissions. The licensed patent will expand the company's efforts by including the scrubbing of $CO_2$.

Contact: Henry Pennline, 412-386-6013


### NETL Honors Researchers with Newly Created Hugh Guthrie Award

NETL has recently created the "Hugh Guthrie Award for Innovation" to honor long-time employee Hugh D. Guthrie. Hugh passed away in February 2007 bringing to a close an engineering career that spanned an incredible 65 of his 87 years. During the past two decades, he worked as senior management and technical advisor to NETL's Strategic Center for Natural Gas and Oil.

The Hugh Guthrie Award provides NETL with an internal vehicle to recognize its reseachers' contributions to the laboratory and to the larger scientific community. Three research teams were honored this year:

- Sofiane Benyahia, Dr. Chris Guenther, Thomas O'Brien, William A. Rogers and Madhava Syamlal for their work on MFIX, an open-source software program that is helping speed commercialization of advanced coal technologies.
- Paul C. Turner, Paul D. Jablonski and Steve Gerdemann, for their contribution to the Armstrong Process, a new low-cost method to produce titanium powder.
- Richard Hammack and others, for their work to develop SEQURE™, the only commercially available technology that can quickly search for expansive oil and gas fields as $CO_2$ storage sites.

Three individuals were also honored:

- Randall Gemmen, for superior leadership in the development and operation of the DOE fuel cell test facility.
- Grant S. Bromhal, for his collaboration with many of NETL's carbon sequestration research partners.
- Dan Sorescu, for his exceptional accomplishments, which have earned three supercomputing awards at various major Department of Defense-shared resource centers.

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## New Capabilities

*Marisa Arnold holding a sample for the Laser Flash Apparatus.*

### New Laser Flash Apparatus Measures Thermal Diffusivity of Materials

NETL recently purchased a Laser Flash Apparatus that can measure the thermal diffusivity of ceramics, metals, composites, refractory materials, and multi-layer systems between room temperature and 1100 °C.

Knowledge of the thermophysical properties of materials and heat transfer optimization of final products is important in developing strategies to protect underlying metallic alloys from extreme environments and/or extreme temperatures associated with advanced fossil energy power systems.

The measurement principle is as follows: The front side of a disk-shaped sample (12.7 mm or 25.4 mm in diameter by 5 mm thick) is heated by a short laser pulse. The heat induced propagates through the sample and the temperature rise is measured as a function of time using an infrared detector. The thermal diffusivity can then be determined using the measured signal.

Initially, the instrument will be used to evaluate thermal diffusivity of refractory liner materials, a critical property impacting gasifier efficiency and refractory wear.

Contact: Marisa D. Arnold, 541-967-5809

*NETL researcher Kirk Gerdes injects a sample into NETL's new gas chromatograph-inductively coupled plasma-mass spectrometer, an analytical instrument that will play an important role in studying the effect of coal contaminants on solid oxide fuel cells.*

### New Measurement Capability for Analyzing Coal Syngas Contaminants

NETL researchers have installed and tested an analytical instrument that will play an important role in studying the effect of coal contaminants on solid oxide fuel cells.

The gas chromatograph-inductively coupled plasma-mass spectrometer offers part-per-billion sensitivity to compounds typically found in trace amounts in coal syngas, including arsenic, phosphorus, selenium, and mercury.The instrument supports fuel cell research at NETL to evaluate the impact on fuel cell performance and degradation of trace species found in coal syngas.

The spectrometer will be mounted into a specially designed mobile test cell and taken to the Wilsonville

Power Systems Development Facility to support fuel cell performance testing on coal syngas scheduled for January 2008.

NETL's research directly addresses high priority goals of the NETL solid oxide fuel cell program, which include evaluating the impact of trace coal syngas species on fuel cell performance and determining efficient methods for mitigation of undesirable effects. The mobile test unit has been designed so that it can support testing at other coal gasification sites, including FutureGen.

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