netlognews

NETL's R&D newsletter *October 2008, Issue 11*

CT Scan Not Only a Medical Technique

NETL Wins Two 2008 R&D 100 Awards

First Measurements at Oxy-Fuel Flame Test Facility

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

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ON THE COVER

Researcher Robert McLendon adjusts the CT scanner used in research at NETL. The scanner is used to measure in situ fluid displacement and sorption of fluids within mineral cores.

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

Medical Technique Adopted to Study Mobility of CO_2 in Coal

Computed tomography – you may be more familiar with the term CT scan – is usually thought of as a medical technique, but researchers at NETL are using CT to assess the potential long-term storage of carbon dioxide (CO_2) in deep, unmineable coal seams.

A paper describing the approach and conclusions has been accepted for publication in the peer- reviewed journal, SPE- Reservoir Evaluation & Engineering- Reservoir Engineering.

CO_2 concentration gradients were determined at the confining and pore pressures of the deep strata. For those evaluating the potential of sequestering CO_2 in such coal seams, this technique provides realistic and essential design information regarding flow and sorption rates and limits of CO_2 sorption. The data can then be used in numerical simulations to predict results for target coal seams.

Researchers are looking at various ways to keep carbon dioxide from getting into the atmosphere. One option for storing carbon dioxide permanently is to inject it into coal seams where it would be trapped inside the coal.

The CT research is used to study the effects of carbon dioxide injection into coal seams, and the implications for additional storage of carbon dioxide. When carbon dioxide is injected into a coal seam, it is sorbed – taken up by the coal through absorption or adsorption and held.

Research performed at NETL on the effects of carbon dioxide sorption demonstrates that under some circumstances sorption can cause the coal to swell and make it more difficult for additional carbon dioxide to be stored.

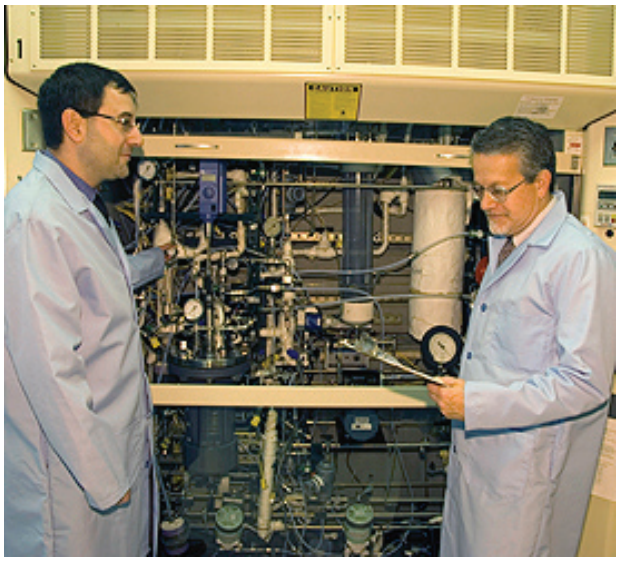
However, NETL research also has shown that carbon dioxide sorption can cause fractures to develop in the coal, which would make the injection easier. This finding apparently has been confirmed by field tests around the world and, in some cases, carbon dioxide injection caused the injectivity to increase.

Contact: Robert McLendon, 412-386-5749

Two Technologies Chosen for 2008 R&D 100 Awards

NETL won two 2008 R&D 100 Awards given each year by R&D Magazine to the 100 most technologically significant products introduced into the marketplace over the past year. The U.S. Department of Energy regards the R&D 100 Awards as an important indicator of the real-world relevance of technologies developed at the national laboratories.

One of the NETL R&D 100 awards is for palladium-based, high-temperature sorbents to capture mercury, arsenic, and selenium. The other is for NETL's Advanced Process Engineering Co-Simulator (APECS) built on the integrated access, workflow, and data services of the ANSYS® Engineering Knowledge Manager™ (EKM).



Evan Granite, left, and Henry Pennline, inventors of the palladium-based high temperature sorbents.

The palladium-based formulations were licensed to Johnson Matthey for commercial development and application to capture mercury, arsenic, and selenium at various stages in the integrated gasification-combined cycle (IGCC) process. Compared with low-temperature capture by activated carbons, capturing these trace elements at high temperature would retain the high thermal efficiency of IGCC plants, which would increase the use of abundant domestic coal reserves.

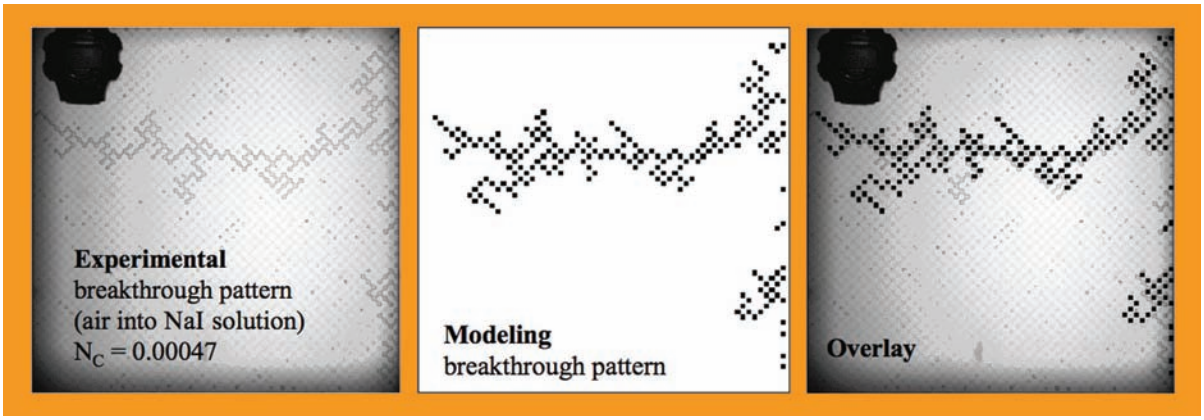
The NETL sorbents are described in U.S. patent 7,033,419 as well as in recent issues of the journals *Industrial & Engineering Chemistry Research* and *Fuel*. Johnson Matthey is a world leader in catalyst manufacture.

APECS with EKM™ is a one-of-a-kind software tool that provides high-fidelity process/equipment co-simulation together with seamless data/model management throughout the energy plant lifecycle, including process innovation, design, operations, and management across the distributed enterprise.

NETL researchers and collaborators from Iowa State University conduct a virtual power plant simulation using NETL's Advanced Process Engineering Co-Simulator (APECS), built on the integrated access, workflow and data services of the ANSYS® Engineering Knowledge Manager.

The process and energy industries can deploy APECS with EKM as a complete engineering solution for fostering rapid technology development, reducing pilot/demonstration-scale facility design time and operating campaigns, and lowering the cost and technical risk in realizing high-efficiency, near-zero emission plants of the future.

Technologies chosen for R&D 100 Awards are voted by an independent judging panel and the editors of R&D. The awards will be presented on October 16 at the R&D 100 Awards banquet in Chicago.



Comparison of modeling with experiment. The figures show breakthrough flow patterns from injection (from the right) of air into a flow cell saturated by a sodium-iodide solution.

Computer Code for Geologic Sequestration Modified for Parallel Computers

Researchers at NETL have modified the computer code NETfLow™ to run on parallel computers, which enable faster computational speeds.

NETL researchers wrote the code, which they use to improve geologic sequestration of carbon dioxide, oil recovery, and other technologies of underground fluid flow.

NETfLow™ is being used to develop new equations for immiscible flow–flow where the fluids are incapable of mixing–through porous media and fracture networks. Immiscible flows occur in such technologies as brinefield sequestration, in which one fluid (e.g., carbon dioxide) displaces another (e.g., brine).

The parallelization involves a rewriting of a previously validated physical model for flow through networks of flow channels. The parallelized code solves the same physical equations as in the previous computer program, but runs much faster, by using computers with parallel processors.

The faster computational speeds allow results to be obtained more quickly, or for larger problems to be studied. For example, on a computer with four processors, the parallelized code runs almost three times as fast as the unparallelized version.

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

Wellbore Cement Research Contributes to EPA Policy on CO_2 Injection

The EPA's recently published proposed rule on carbon dioxide injection into wells has cited the work of NETL researchers on the alteration of cement under a sequestration scenario. The NETL work has shown that corrosion of cement is likely to be very limited, and therefore not lead to failure in a properly completed well. NETL's results are in general agreement with the limited field evidence that is available. Previous laboratory experiments by other laboratories have overestimated the impact of chemical corrosion, likely due to experimental conditions that do not match the typical field conditions.

The NETL work is cited in the proposed rule, "Federal Requirements Under the Underground Injection Control (UIC) Program for Carbon Dioxide (CO_2) Geologic Sequestration (GS) Wells." The NETL team has recently published its second in a series of articles in Environmental Science & Technology, which presents NETL's results.

Contact: Brian Strazisar, 412-386-5988

NETL researcher Kelly Rose, left, and Dr. Jang Jun Bahk of Korea Gas Corporation examine hydrate bearing sediments from a recent Korean gas hydrate expedition in the Ulleung Basin, South Korea.

Methane Hydrate Researchers Complete Marine Expedition Off Cascadia Margin

NETL researcher Kelly Rose provided shipboard sedimentological and core processing support and NETL methane hydrate graduate research fellow Laura Lapham participated as a key member of the shipboard geochemistry team on the recently completed three-week ocean expedition near Vancouver Island off the British Columbia coast. The expedition sought to characterize and better understand the role of gas hydrate bearing sediments in the region. In particular, the expedition off the Cascadia margin focused largely on seafloor stability and climate-related issues. The expedition was led by the Geological Survey of Canada and included researchers from the United States Geological Survey, McGill University, and DOE. Rose will also be conducting post-expedition petrophysical, xrd/xrf, and particle-size analyses of key sediment samples for further interpretation and integration with the geophysical, geochemical, and physical properties datasets. Lapham plans to analyze sulfate profiles from each of the sites studied during the project.

During the expedition aboard the Canadian Coast Guard ship The Tully, over 1,800 samples and more than 100 kilometers of geophysical surveys were collected. (Full story of NETL Methane Hydrates research here.)

Contact: Kelly Rose, 304-285-4157

NETL Sheds New Light on Unique Class of CO_2 Capture Materials

Scientists in NETL's Office of Research and Development have developed an experimental technique that provides a better evaluation of storage capacity for a new CO_2 capture material, a nickel based metal-organic framework. The technique relies on an optical phenomenon called attenuated total reflectance and when used with infrared light is capable of probing the near surface region of porous solids. The real power of this technique relies on its ability to differentiate between captured CO_2 molecules and those in the gas-phase. It is also capable of probing changes that occur in the crystalline structure of the capture material as a result of exposure to CO_2. Using the attenuated total reflectance measurement, NETL researchers were able to directly show, for the first time, that structural changes are responsible for the high CO_2 capture capacity of a new nickel based metal-organic framework. Furthermore, the measurements provided evidence for a particularly strong interaction between CO_2 and the pore of the capture framework. These new experiments provide critical information on the CO_2 storage process and provide a molecular level understanding that will enable computational chemists to model new capture materials.

Contact: Angela Goodman, 412-386-4962

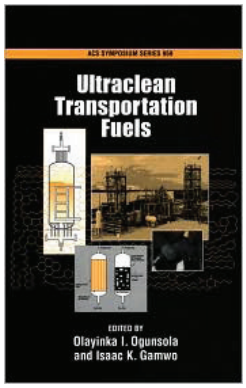
During recent helicopter electromagnetic surveys in Wyoming, ground conductivity was measured by the sensor suspended from the helicopter. Survey data will be used in mapping soil and geologic properties for environmental studies for managing produced water from coal bed natural gas production.

Helicopter Electromagnetic Surveys Completed in Powder River Basin

FUGRO Airborne Surveys, Inc., which conducts airborne surveys under contract to NETL, completed a helicopter electromagnet survey over two study areas in the Powder River Basin in June. The Powder River Basin is an area of 14 million acres in northeastern Wyoming and southeastern Montana and produces oil and coalbed natural gas. NETL is using airborne and ground-based geophysical methods to develop improved strategies for managing coalbed-natural gas (CBNG) produced water. The survey received quality assurance/quality control oversight by the U.S. Geological Survey through a cooperative agreement between NETL and USGS. Project partners include the Wyoming Department of Water Quality, the U.S. Bureau of Land Management, Anadarko Petroleum Corp., BeneTerra LLC, and West Virginia University Natural Resource Analysis Center.

The recent survey included a proposed subsurface drip irrigation (SDI) site that will receive CBNG produced water, and the flood plain of Beaver Creek, a tributary of the Powder River that is being considered for CBNG-produced water discharges under provision of Wyoming's Agricultural Use Protection Policy, Section 20. Information from the helicopter electromagnet survey will be used to design the SDI system so that areas of low permeability, salt lenses, and high total dissolved solids groundwater are avoided. These data also will be used to determine the suitability of sub-irrigated land on the Beaver Creek flood plain for CBNG discharges. Both projects have the potential to increase CBNG production by providing beneficial and environmentally benign uses for produced water.

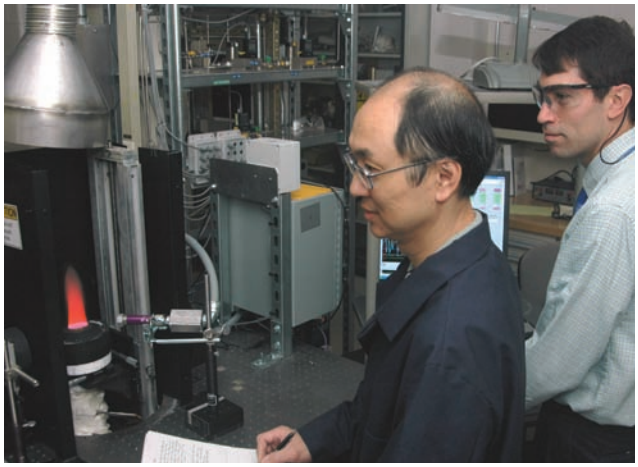
Contact: Jim Sams, 412-386-5767



Book Makes ACS Top Ten Best-Seller List

"Ultraclean Transportation Fuel," a book co-edited by NETL's Dr. Isaac K. Gamwo and Dr. Olayinka I. Ogunsola, a program manager in the DOE Fossil Energy Office of Oil and Natural Gas, made the top ten best-seller list in American Chemical Society's (ACS) publications. The ACS publications division maintains a list of over 500 books and is viewed around the world by scientists as the best single source for published information on chemical research. The ACS tracks the trajectories of their books' ratings by analyzing peaks and falls in book sales. The book was sponsored by the ACS Division of Fuel Chemistry and was published by Oxford, the world's largest University press. Dr. Gamwo and several other NETL researchers wrote multiple chapters in the book, which delivers outstanding research topics in synthetic and hydrocarbon fuels.

Contact: Isaac K. Gamwo, 412 386-6537



Joe Yip, left, and Ben Chorpening, researchers in NETL's Office of Research and Development, prepare to conduct an experiment in NETL's unique oxy-fuel flame test facility. The color of the oxy-hydrogen flame is due to the presence of steam.

NETL Researchers Take First Measurements at Oxy-Fuel Flame Test Facility

Researchers at NETL are not quite trying to start a flame underwater and keep it burning, but some of their recent research isn't far from that.

Energy System Dynamics Division researchers have taken their first measurements of an oxy-hydrogen flame in our unique oxy-fuel flame test facility where the amount of steam may be as high as 70 percent of the input gas. Obtaining data under these conditions is important in understanding the issue of trying to light and sustain a flame in the presence of that much steam.

Oxy-fuel combustion schemes are being considered as a mitigation strategy to more efficiently reach the goal of zero emissions of carbon dioxide (CO_2) from combustion of fossil fuels. This approach is attractive because the major products of combustion in oxy-fuel systems are CO_2 and water. CO_2 can be separated simply by cooling the combustion products to condense out the water, yielding a concentrated CO_2 stream for subsequent sequestration.

Since nitrogen is removed from air to produce oxygen for the oxy-combustion, a diluent (diluting agent) such as steam, CO_2, or flue gas (steam plus CO_2) must be added to prevent overheating these hydrogen-oxygen flames. Since 80 percent of regular air is nitrogen, which has a heat capacity that affects the flame temperature, the temperature would be higher without the nitrogen.

In some cases, added diluent such as steam can represent up to 70 percent of the volume of the input gas flow to the burner. The studies provide valuable information about lighting and sustaining a flame in such a high steam environment.

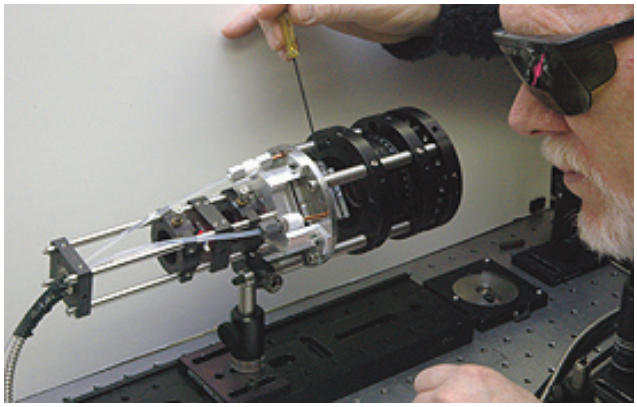
Little data is available in the literature to enable design of oxy-fuel combustion systems. The successful testing at NETL represents an important step toward the goal of measuring flame speeds and radiative properties of these flames, which are needed to accurately simulate and design advanced power systems for carbon sequestration.

Contact: Joe Yip, 304-285-5434

Hydro-gasification Model Used as Design Tool

NETL's Computational Science Division has been providing computational fluid dynamics support to Arizona Public Service (APS) to aid in the development and design of a bench-scale hydrogasifier. APS provided NETL with a simulation matrix, which explored the effect of hydrogen nozzle inside diameter, nozzle vertical angle, and swirl under various coal and hydrogen feed rates. Working jointly, APS and NETL post-processed these simulation results using statistical software and standard CFD tools to evaluate the response of solids mixing, solids flux, and gas temperature at four different elevations in the reactor. These response variables were selected to minimize recirculation in the vicinity of the hydrogen nozzles and maximize gas-solids mixing through the reactor. The analysis showed the bench-scale gasifier should be designed and operated with a large hydrogen nozzle inside diameter, at an angle of 45 degrees to the vertical and with 30 degrees of swirl. APS is in the final phase of its design process, and these CFD results have been incorporated into the design specifications.

Contact: Chris Guenther, 304-285-4483



Inventor Steven Woodruff of the Energy Systems Dynamics Division demonstrates laser spark plug system.

Laser Spark Plug Patented

Recently, a patent was granted for a laser spark system (Patent No. 7,421,166) invented by researchers Steven Woodruff and Dustin L. McIntyre. The laser spark distribution and ignition system reduces the high power optical requirements in a laser ignition and distribution system, allowing the use of optical fibers to deliver low-peak energy-pumping pulses to a laser amplifier or laser oscillator. An optical distributor distributes and delivers optical pumping energy from an optical pumping source to multiple combustion chambers incorporating laser oscillators or laser amplifiers to induce a laser park within a combustion chamber. The laser spark generators produce a high-peak-power laser spark, from a single low-power pulse.

The laser spark plug enables natural gas-fired engines to be operated at higher compression ratios and leaner fuel/air ratios that result in lower NO_x emissions than with conventional electrical spark plugs. The target market for this ignition system is natural gas-fueled reciprocating engines used for pumping and power generation. It also has potential use for other ignition needs including gas turbine engines and can be applied to the Laser Induced Breakdown Spectroscopy sensor devices. The laser spark plug was tested in NETL's Ricardo single-cylinder engine in December 2007.

Contact: Steven Woodruff, 304-285-4175

Research Data Aids Clean-up of Allegheny National Forest

Over the weekend of August 16, 2008, vandals opened valves on seven crude oil storage tank batteries in Corydon and Hamilton townships, McKean County, PA, causing an estimated 36,000 to 45,000 gallons of crude oil to flow from the storage units. About half of the crude oil made its way to the North Branch of Chappel Fork, which flows into Chappel Bay of the Allegheny Reservoir. The U.S. Forest Service reported that the spill killed three beavers in addition to many fish along six miles of impacted stream. As part of the EPACT program, NETL has been monitoring the benthic macroinvertebrate populations monthly in a number of streams within the Allegheny National Forest (ANF) to evaluate the potential impact of future oil and gas activities. One such site is located on Chappel Fork, below the location of the current spill. NETL is coordinating activities and providing results to the U.S. EPA, the Pennsylvania Department of Environmental Protection, and ANF personnel involved in site clean-up and assessment.

Contact: Hank Edenborn, 412-386-6539

NETL's Virtual Power Plant Co-Simulation R&D Presented at Coal Conference

NETL, Iowa State University (ISU), and Ames Laboratory highlighted recent R&D activities in virtual power plant co-simulation at the 33rd International Technical Conference on Coal Utilization and Fuel Systems (the Clearwater Coal Conference). The presentation discussed ongoing collaborative efforts to integrate NETL's Advanced Process Engineering Co-Simulator (APECS) with VE-Suite, an open-source virtual engineering (VE) software toolkit, developed at ISU and Ames Lab. The presentation described the integration of overall power plant data with high-fidelity computational fluid dynamics (CFD) results from APECS process/CFD co-simulations accessed via the ANSYS Engineering Knowledge Manager. Using virtual power plant co-simulations will let designers

of next-generation fossil energy plants develop and test cutting-edge technologies more quickly than in previous decades.

Contact: Stephen E. Zitney, 304-285-1379

Journal Paper Details CO_2 Capture Membranes

The *Journal of Membrane Science* recently published a paper detailing NETL's development of a new class of CO_2 selective membrane for which a provisional patent has been issued. Results shown in the paper are particularly important because they represent the development of a facilitated transport membrane not dependent on an aqueous transport phase. Aqueous phase membranes tend to fail at high temperature due to evaporation of the transport medium, and, as a result, the development of the NETL membrane represents a major step forward in high temperature CO_2 selective membrane development. The membrane consists of an ionic liquid that has the capability to form chemical complexes with CO_2 and a high temperature polymer support. The ionic liquid was developed under a Cooperative Research and Development Agreement with the University of Notre Dame.

Contact: David Luebke, 412-386-4118

NETL Researchers Test First Active Combustion Throttle Valve Body Designs

A team of engineers from NETL and the University of Pittsburgh recently produced and tested two Active Combustion Throttle (ACT) prototype valve bodies. Conceived by NETL and originally intended for balancing fuel flows for gas turbines, the ACT concept is being developed for use in any gas-burning system for flow balancing or for high-speed fuel flow modulation (for active combustion control) of single burners – especially in variable-fuel (fuel-flexibility) applications. The ACT concept involves using a fast-acting control valve to modulate fuel flow in a combustor to control emissions and improve combustion stability. The ACT concept was conceived by NETL and subsequently patented by NETL with the University of Pittsburgh.

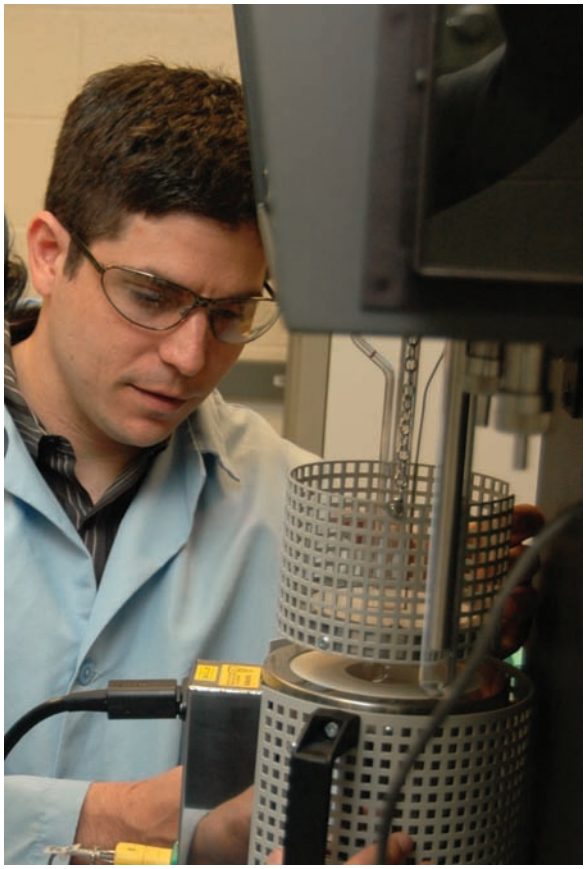
The ACT valve bodies were fabricated at the University of Pittsburgh from acrylic using Computer Numerical Control (CNC) fabrication methods. They were tested as part of NETL's University Research Initiative at NETL combustion facilities to determine their valve (flow) coefficients over the designed range of motion of the control actuator. The two designs offer the options of either fast-opening valve behavior for high-speed combustion instability control, or a slower-opening behavior for more gradual flow control. The throttle bodies and the electromagnetic actuator components that will ultimately drive the control elements have been developed separately to this point. The first integrated (valve body and control actuator) prototypes should be ready for fabrication and testing within the next two months.

Contact: J. Peter Hensel, 304-285-4073

Paper Published on Noble Metal Catalysts for Oxidation of Mercury in Flue Gas

NETL studies on materials proposed as catalysts for oxidation of mercury are summarized in an invited paper, "Noble Metal Catalysts for Mercury Oxidation in Utility Flue Gas," published in the July 2008 issue of *Platinum Metals Review*. These materials include palladium, gold, platinum, SCR catalysts, fly ash, Thief carbons, and activated carbons. A bench-scale packed-bed reactor was used to study the oxidation of mercury using gold, platinum, and palladium catalysts. While gold, palladium, and platinum all exhibited good initial activity for mercury oxidation, there were significant differences in behavior relative to catalyst deactivation over time, poisons, and chlorine storage capabilities. This information, along with differences in the commodity prices of the metals, can help utility management make good decisions for the choice of catalyst to be installed upstream of a wet scrubber.

Contact: Evan J. Granite, 412-386-4607



Christopher Matranga prepares an experiment that will use a specialized chemisorption analyzer to characterize the catalytic properties of a novel class of nanocatalysts.

American Scientific Publishers (ASP) Enlists NETL Expertise on Nanotechnology

An NETL researcher, Dr. Christopher Matranga, authored a chapter titled "Gas Interactions with Carbon Nanotubes" for the newly released ASP publication, Chemistry of Carbon Nanotubes. The single-author chapter focuses on the chemistry of carbon nanotubes and their use for separating gases such as carbon dioxide and hydrogen. Researchers here have been actively developing and applying nanotechnology to improve syngas conversion catalysts and CO_2 separation membranes for fossil energy systems. The 3-volume publication includes 39 state-of-the-art reviews by more than 90 leading experts from 20 countries.

Contact: Christopher Matranga, 412/386-4114

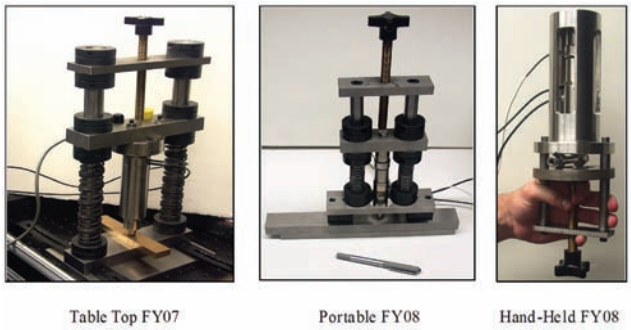
NETL, WVU Collaborate to Produce New Analytical Device

Researchers at NETL and West Virginia University (WVU) just created a portable micro-indenter that can provide non-destructive analysis of properties of a variety of materials.

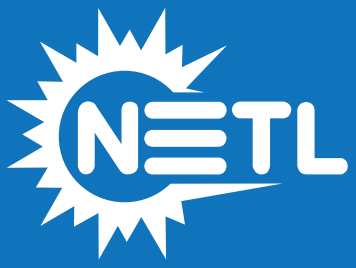
Mary Anne Alvin of NETL's Materials and Component Development for Advanced Turbine Systems project, along with Dr. Bruce Kang, Dr. Tong Feng, and Mr. Jarred Tannebaum of WVU, developed not only the methodology, but also a series of micro-indentation systems to determine the stiffness of metals, superalloys, single crystal matrics, and coated material systems. Destructive analysis was previously used to determine these properties.

The collaborators originally developed a tabletop unit, and more recently have developed portable and hand-held units. The newly developed portable unit makes testing easier in either the research laboratory setting or at field sites. The unit can be used with flat, tubular, or curved architectures.

Contact: Mary Anne Alvin, 412-386-5498



The three types of micro-indentation systems.



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