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netlog

The NETL newsletter

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Christopher Matranga, right, and Neetha Khan, a post-doctoral research associate, prepare an experiment in NETL's Omicron Analysis and Surface Imaging System. The OASIS system allows researchers to image individual atoms and determine the elemental composition of the first few atomic layers of surfaces relevant to fossil energy applications.

NETL Conducts Groundbreaking Research on Syngas-producing Nanocatalysts.

Researchers in the Chemistry and Surface Science Division in the Office of Research and Development have completed a detailed study of a novel nanocatalyst with enhanced capabilities for producing syngas.

The NETL research focused on catalysts consisting of a barium hexa-aluminate support embedded with platinum nanoparticles.

Previous work has shown that with 20 times less platinum, these nanocatalysts yield approximately 5 times as much syngas from the partial oxidation of methane as do traditional alumina-supported catalysts.

The work is part of an ongoing collaboration with faculty in the Chemical Engineering Department at the University of Pittsburgh. Portions of the research were submitted for publication in the *Journal of Physical Chemistry.*

Contact: Christopher Matranga, 412-386-4114

Scientists to Produce Penetrators for Use in Ballistic Testing by the Army

NETL scientists will produce ballistic penetrators for the Army Research Laboratory's Armor Mechanics Branch in Aberdeen, MD. The penetrators are critical to the performance testing of new armor applications that will protect soldiers and military systems being fielded throughout the Army's areas of operations. The Army laboratory has tried unsuccessfully to have these penetrators produced elsewhere. Army Research Laboratory officials say NETL's unique materials capabilities make it the only place where this work can be done.

Contact: Paul Turner, 541-967-5863

Ranjani Siriwardane of the Separations and Fuels Processing Division in the Office of Research and Development has done extensive R&D on sorbents to remove carbon dioxide.

NETL Reports First Regenerable Warm Gas Temperature Carbon Dioxide Removal Sorbent

Researchers have reported the first regenerable sorbent that can remove carbon dioxide at warm gas temperatures during the coal gasification process. Currently, no regenerable carbon dioxide removal sorbents are available for the gasification process at warm gas temperatures, from 200 to 400 °C. The commercially available processes require gas cooling, which contributes to a loss in thermal efficiency. The NETL-developed sorbent can be utilized without cooling the coal gas. This sodium-based sorbent shows very high carbon dioxide capture capacity and greater than 99% carbon dioxide removal efficiency at 315 °C. The sorbent can be regenerated at 700 °C.

A 10-cycle test conducted at NETL showed that the capture capacity increased during the cyclic testing.

The sorbent also is described in a peer-reviewed paper, "Novel Regenerable Sodium Based Sorbents for CO_2 Capture at Warm Gas Temperatures" that has been accepted for publication in *Energy and Fuels* journal.

A patent application for this NETL-developed sodium-based sorbent process is under review in the U.S. Patent office.

Contact: Ranjani Siriwardane, 304-285-4513

NETL-developed refractory (right) showing improved performance over conventional commercial refractory (left).

NETL-Developed Refractory Licensed to Company for Production

Harbison-Walker Refractories Company, a major manufacturer of refractory products, is producing a refractory developed by NETL and marketing the product for gasification applications under the product name of Aurex® 95P. The company was granted an exclusive license for the production of this refractory composition, which will extend the service life of slagging gasifiers.

The gasifier industry has identified refractory service life as a key barrier to widespread acceptance and commercialization of gasification technology. Current commercial refractories installed in air-cooled slag¬ging gasifiers fail in as little as three months in high-wear areas of the gasifier and last no longer than two years in the least demanding locations. Costs related to a failure of the refractory lining are high, both in terms of material replacement (as high as $1 million) and lost production due to gasifier shutdown. Improved refractory linings will increase the reliability and online availability of gasifiers, helping to move this technology forward in the marketplace.

Research at NETL improved the high-temperature performance of refractory materials, first by analyzing failure modes of refractories in gasifier service, and second by formulating improved compositions that withstand the identified failure mechanisms. This resulted in the development of a high-chromium/alumina matrix refractory modified with phosphate, which was patented by NETL (U.S. Patent number 6,815,386). From the laboratory, the refractory composition was scaled up and field tested in numerous gasifiers around the country. Based on postmortem analysis of field trial material, the phosphate-containing refractory was found to reduce or eliminate spalling wear, resulting in a service life improvement estimated at approximately 50 percent over conventional refractory materials. The patented refractory also was found to have equivalent or better resistance to chemical deposition, the other main wear mechanism impacting gasifier service life.

Contact: Cindy Powell, 541-967-5803

NETL Licenses Sorbents

NETL has licensed our palladium-based sorbents, invented by researchers Evan Granite and Henry Pennline, for high-temperature capture of mercury, arsenic, and selenium from fuel gas to Johnson Matthey, a specialty chemicals company. Johnson Matthey will be responsible for commercial development and application of the sorbents. The sorbents address the need for a low-cost mercury removal technique that can be applied to integrated gasification combined-cycle (IGCC) and coal-burning power plants.

The sorbents are described in U.S. Patent number 7,033,419, issued in April 2006, and in a recent publication in *Industrial & Engineering Chemistry Research*. Gasification is an important strategy for increasing the utilization of abundant domestic coal reserves. High-temperature capture of the trace elements mercury, arsenic, and selenium helps preserve the high-thermal efficiency of integrated IGCC plants versus low-temperature capture by activated carbons.

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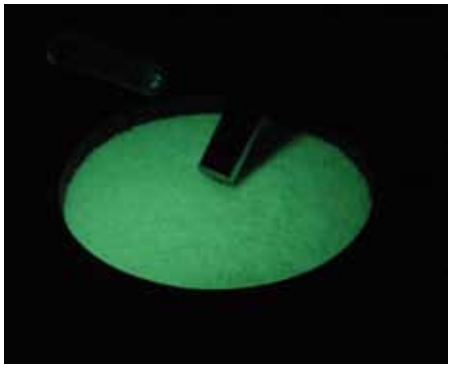


Phosphorescent plastic beads glowing on the bench

Tests Simulate Penetration of a Coal Jet Injected Into a Transport Gasifier

In many proposed coal-fueled advanced electric power plants, the coal reacts with oxygen and steam in a device called a transport gasifier. This gasifier converts the solid coal into a gaseous fuel, which is then further processed to remove pollutants and undesirable chemical compounds. The result of this processing is a fuel that can be used to generate electricity and has very little adverse impact on the environment.

Advanced technology developer KBR is actively researching transport gasifier technology at a commercial scale under DOE's Clean Coal Power Initiative and at a smaller scale at the Power System Development Facility (PSDF). Proper operation of KBR's commercial-scale gasifier depends on the correct distribution of coal into the gasifier. Tests conducted at the smaller PSDF may not accurately predict the larger commercial-scale behavior. The commercial-scale system has a cross-sectional area 25 times larger than the area at the PSDF. To aid in this development effort, NETL is conducting computer simulations of the commercial gasifier with various coal-feed configurations to predict the mixing patterns across this area. To help establish the credibility of these simulation results at high-temperature and -pressure gasifier operation, NETL researchers are using their facility to conduct additional simulations that resemble a commercial system. While these tests are conducted at the same fluidization regimes as those envisioned for the commercial unit, they are not conducted at the same high temperature and pressure that would be used in a commercial unit. Instead, the NETL facility operates at room temperature and low pressure, and hence these tests are called cold-flow tests.

For these tests, 0.75-mm phosphorescent polyethylene beads are continuously injected into the equipment while the same material flows upward past the injection port at over 40,000 kg/hr. This section of the equipment is called the riser. The injected beads, which form a jet as they are forced into the riser, are exposed to UV light and induced to glow just before they enter the riser. Once inside the riser, the glowing beads can be located and their concentrations determined using photosensors, which are placed in the flow field. Additional fiber optic and piezoelectric probes are used to characterize the resulting overall flow structure and the effect the jet of injected solids has on the circulating material. Using these techniques, jet behavior has been observed for variations in both riser and jet-operating conditions. These measurements have provided a wide range of data that will be compared with the results of the computer simulations to instill more confidence in those results.

Contacts: Lawrence Shadle, 304-285-4647 and Christopher Ludlow, 304-285-4608

Specialty Metals Processing Consortium Program Planning Meeting Hosted by NETL

The Specialty Metals Processing Consortium (SMPC) board of directors and the associated member companies' vice presidents of technology met at NETL on May 17 to develop a strategy for cooperative superalloy processing research. The SMPC is a consortium of reactive metals and nickel superalloy producers with primary markets in land- and air-based gas turbines and other high-temperature and extreme environments. The technical meeting included representatives from Carpenter Technologies of Reading, PA; Special Metals of Huntington, WV; Timet of Dallas, TX; and ATI Allvac of Monroe, NC. Also present were representatives of Sandia National Labs. Discussions were held to define how the SMPC, its member companies, and NETL can better collaborate on research topics of interest. Discussions centered on the progress of planning for the proposed research program. Further discussions were held on methodologies for obtaining third-party funding to complement ongoing research efforts within the SMPC and NETL. The heart of the research being proposed is better instrumentation and melting practices to obtain larger superalloy ingots with fewer defects. As gas turbines increase in size and efficiency, larger superalloy ingots will be required in order to fabricate essential high-temperature components. Currently, superalloy ingot size is limited to about 24 inches in diameter due to defects generated during solidification.

Contact: Paul King, 541-967-5948

NETL researchers Sophie Bullard, Bernie Covino, and Steve Matthes (left to right) install a new corrosion sensor during the 5-month field trial.

Power Plant Field Test Completed to Monitor Fireside Corrosion

NETL has successfully completed a five-month field test of electrochemical corrosion rate sensors in a waste incineration power plant. The plant, which is operated by Covanta Marion Inc. (a Covanta Energy Company), is located in Brooks, OR. Air-cooled corrosion sensors, designed and built at NETL, were placed in four locations of a boiler at the location and depth of the waterwall. Two different sensor alloys were used: SA178A, the material used in the waterwall, and UTP6222, the weld overlay rod used to apply an Inconel 625 overlay. Sensors were replaced after intervals of one to two months in order to study their degradation and replace the thermocouples. Initial results show that this technology was able to follow changes in corrosion due to process changes such as startup and shutdown. Further analysis of the data will help determine if electrochemical corrosion rates can be calibrated against mass loss measurements of the sensors and if future tests should include automatic control of sensor temperature to match waterwall temperatures. This technology represents a tool for power plant operators to monitor degradation of boiler components and use corrosion rate as a process variable.

Contact: Bernie Covino, 541-967-5828

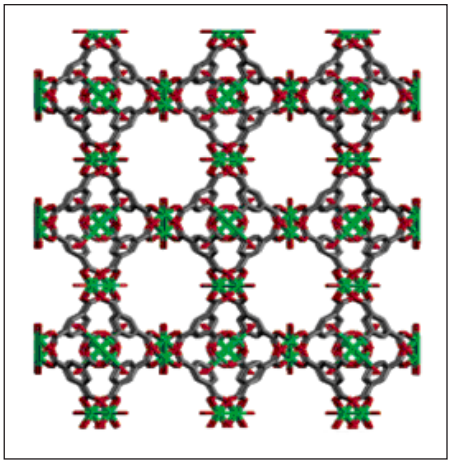
DOE Transfers Steel Casting Technology to Rock Island Arsenal

A steel casting technology developed by DOE has been transferred to the U.S. Army's Rock Island Arsenal to manufacture improved armor for vehicles used in the global war on terrorism.

NETL provided the Rock Island Arsenal with process guidelines, parameters, expertise, and patterns to set up and operate a facility for making steel castings using an NETL-developed process called loose-bonded sand, lost-foam technology. The facilities at the arsenal, in Rock Island, Ill., will be used to produce the improved cast steel armor plating for Army vehicles.

For the full story, click here.

Contact: Paul Turner, 541-967-5863



View of CuBTC showing open nano-channels

Metal Organic Frameworks Proven Effective for Adsorption of Hydrogen and CO_2 Gases

New research has demonstrated that the promising new materials called MOFs, or Metal Organic Frameworks, may be better at gas adsorption than previously thought. These recently developed MOFs are constructed from metal ion clusters and simple organic linker molecules. Their very regular crystalline nature, high surface area, and large porosity combine to make them ideal agents for adsorbing gases such as hydrogen or carbon dioxide. A prime example of this class of material is the MOF with the chemical formula $Cu_3(BTC)_2$. The new work has uncovered better methods for both synthesizing and activating this material so that it attains its full capacity for storing gases. The new experimental data allow fair comparison with new theoretical simulations of the same gas adsorption process that were also a critical part of this study. The simulations included exploration of subtle chemical effects. For example, quantum effects were found to play a major role in the adsorption of hydrogen at low temperatures. This has important implications for the theory of the adsorption when applied to low molecular weight gases such as hydrogen or deuterium. The entire study was a collaborative effort by NETL, the University of Pittsburgh, Advanced Materials Corporation, and the University of Trento, Italy. The study is fully described in a paper recently accepted for publication by the highly regarded Journal of Physical Chemistry.

Contact: Bradley Bockrath, 412-386-6081

Model Developed for Chromia Evaporation from Alloys During Service at Elevated Temperatures

Many alloys used in fossil energy power generation systems are protected from the hostile service environment by the formation of chromium oxide (Cr_2O_3) surface scales. While stable in dry air environments at temperatures as high at 900 °C, chromium oxide can evaporate in moist air and steam environments at lower temperatures. This can lead to significant material wastage. NETL scientist Gordon Holcomb has developed a model for the reactive evaporation of chromium oxide that incorporates the effects of air or steam temperature, pressure, velocity, oxygen content, and water content. Experiments are planned to verify this model using an NETL autoclave that will allow for the exposure of alloys to high-temperature and high-pressure steam with controlled dissolved oxygen contents.

The model accurately predicts observed material loss at 760 °C in a Cr_2O_3 forming nickel-base alloy, Haynes 230, in air containing 37% H_2O water vapor flowing at $2.2x10^{-3}$ m/s and $5.6x10^{-3}$ m/s. The model was also used to evaluate the evaporation rate of Cr_2O_3 under various steam turbine conditions. The analysis showed that at pressures and temperatures (~ 600 °C and 30MPa) representative of current advanced steam plants, minimal evaporation occurs. However, at the higher steam temperatures and pressures projected for advanced power systems, the model indicates that evaporation could be significant. In that case, evaporation would have to be controlled by selecting alloys with elements that lower Cr activity; using coatings to reduce metal temperatures and increase the diffusion boundary layer; and/or controlling steam chemistry to reduce dissolved oxygen.

Contact: Gordon Holcomb, 541-967-5874

Researchers Use Advanced Model for Coal Swelling and Shrinkage to Interpret Carbon Dioxide Sequestration Field Project

NETL researchers are advancing the interpretation and use of field-project data for carbon dioxide sequestration in coal seams. Using their advanced model, NETL researchers completed a study on the combined influence of various coal parameters on swelling and shrinkage. A three-dimensional model was developed to study the influence of these parameters. Coal shrinkage and swelling are considered to be potential problems during carbon dioxide sequestration. These effects occur when methane is produced from, or carbon dioxide is injected into, a coal seam.

The model is based on constitutive equations that account for the coupled fluid pressure-deformation behavior of a porous medium that undergoes swelling and shrinkage. Data from the field project of the Allison unit located in the San Juan basin were interpreted with the model. The interpretations reveal, for example, that a value of 521,000 psi for Young's modulus should be used for future design calculations in the San Juan basin. A paper titled "Influence of Shrinkage and Swelling Properties on Geologic Sequestration of Carbon Dioxide" is contained in the Proceedings of the International Coalbed Methane Symposium, Tuscaloosa, AL, May 21-25, 2007, and was presented at the meeting. Click here for the paper and here for the presentation.

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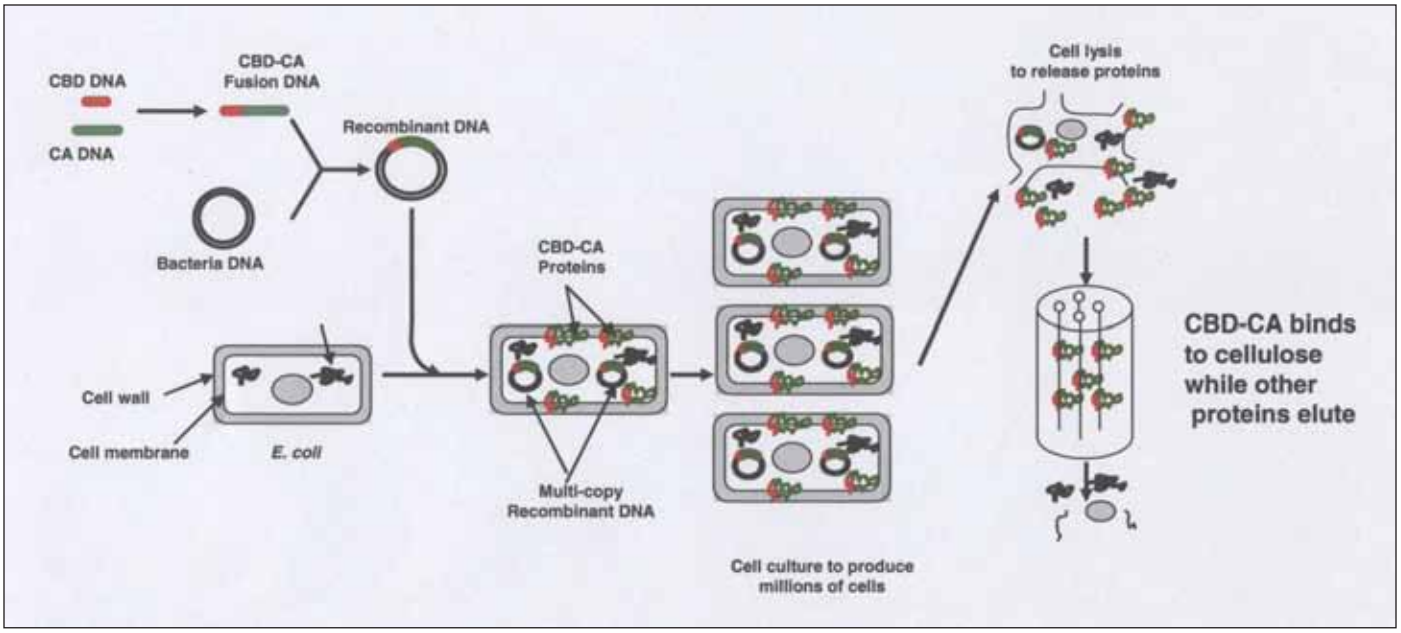


Simplified schematic of the production of carbonic anhydrase with cellulose-binding domain.

Patent Application Filed on CO_2 Capture Technique

NETL filed a patent application for a carbon dioxide capture technique with the potential for large-scale application in the power industry. The invention also could be used in other industries that utilize carbonic anhydrase (an enzyme that catalyzes the removal of water from a compound)-based technologies to capture carbon dioxide. NETL researchers developed the technique jointly with researchers at the University of Pittsburgh. The invention is a novel genetic engineering technique resulting in the creation of a hybrid carbonic anhydrase enzyme with an attached cellulose-binding domain. This allows production and purification of large quantities of the enzyme at very low cost (estimated at dollars per kilogram), as well as achieving spontaneous immobilization on inexpensive support materials.

Contact: Robert Dilmore, 412-386-5763

Baseline Monitoring Survey Completed at San Juan Basin Pilot Injection Site

Faults and fractures were characterized at the San Juan Basin in the vicinity of a planned CO_2 injection site, and a grid was established for monitoring storage integrity in the near-surface. The San Juan Basin project is a pilot-scale injection of CO_2 into a coal seam in Northwestern New Mexico to study carbon sequestration as well as enhanced coalbed methane recovery. Injection is scheduled to begin late in 2007. The overall activity is part of the Southwest Regional Partnership on Carbon Sequestration. Results of this work were presented at the Sixth Annual Conference on Carbon Capture and Sequestration.

Baseline measurements over this grid included background tracer levels, CO_2 surface flux and isotopes, soil gas hydrocarbon levels, and electrical conductivity in the soil. Baseline characterization is critical to the interpretation of monitoring results that NETL will obtain once injection begins. In addition, several locations on the grid have exhibited hydrocarbon microseepage to the surface, indicating that those locations should be monitored more closely as the project proceeds.

Contact: Brian Strazisar, 412-386-5988

New Capabilities at NETL

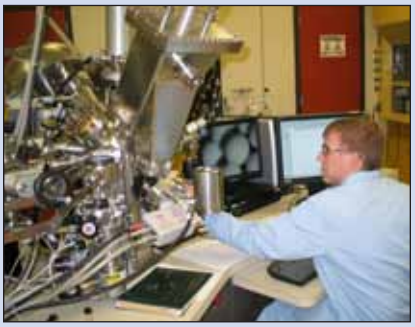
Steve Woodruff, of the Energy System Dynamics Division, Runs an experiment with the new laser

Nd:YAG Laser Enhances Diagnostics Capabilities

NETL has enhanced the capabilities of its Laser Spectroscopy Laboratory through the recent acquisition of a more powerful Nd:YAG laser. Nd:YAG lasers are among the most common types of lasers but have a variety of applications.

Researchers in NETL's Office of Research and Development intend to use the laser to generate a detailed data set of flame properties to support NETL's combustion modeling efforts. ORD researchers have conducted experiments using methane and/or hydrogen as a fuel to explore the combustion properties of turbulent flames.

Contact: Peter Strakey, 304-285-4476



John Baltrus, of the Chemistry and Surface Science Division, performs an analysis using the upgraded spectrometer.

NETL Upgrades Surface Analysis Instrument

The X-ray photoelectron spectrometer, located in the Chemistry and Surface Science Division, has been upgraded by installing a new computer and computer-control interface. The instrument is used for studies of the chemical composition of material surfaces. NETL researchers use it to help understand the behavior of membranes used for hydrogen separation, sorbents for mercury capture, and sorbents for carbon dioxide capture and sequestration.

The upgrade included the installation of sophisticated data-handling software that will improve both the amount and the quality of information NETL researchers can extract from measurements made using the instrument. The upgrade also will extend the useful lifetime of the instrument.

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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.