netlog

NETL's R&D newsletter

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ON THE COVER

Dr. Bryan Morreale stands next to the test rig used for studying the effects of coal and biomass mixtures on gasification products.

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.

Co-Gasification—Researchers Combine Coal and Biomass

NETL researchers are looking at ways that we can combine the natural resources of coal and biomass – biomass including such growing things as wheat straw, corn stover, switchgrass, mixed hardwood and distillers' dried grains with corn fiber, and even algae – but avoid the emission of carbon dioxide.

The researchers are studying a process called co-gasification in which various types of coal and biomass are put together and converted into a gaseous product stream that can be used to produce electricity, hydrogen, chemicals and liquid transportation fuels.

What about the carbon that resides in coal and biomass? Doesn't it manage to escape into the atmosphere?

"No," explains researcher Bryan Morreale in the Chemistry and Surface Science Division of NETL's Office of Research and Development. "With the blending of biomass and coal in the co-gasification process, you decrease the environmental impact because biomass is carbon neutral. If you apply carbon sequestration technologies, you actually have a process that's carbon negative – it consumes the carbon."

The process produces a product stream called synthesis gas, which has great flexibility to be used in several ways. That flexibility is one of the advantages of the co-gasification process; another advantage is the contribution to our national security through utilization of an abundant natural resource without environmental consequences.

"Coal is one of the most abundant resources we have. With extensive use of co-gasification, we would reduce our dependence on foreign oil," Morreale notes.

NETL's research focuses on energy crops, not food crops. Because co-gasification can use any biomass to produce the synthesis gas, there is no need to develop a particular energy crop. Existing mixed prairie grass, forest residues, waste-wood, and even various waste streams can be converted to synthesis gas. The advantage with co-gasification using coal is that the steady supply of coal supplies a baseline that can be supplemented by biomass whenever available.

“Energy and food are two of our most important national needs,” Morreale says to explain the focus on non-food crops. “If we don’t have food we can’t live.”

The energy crops – wheat straw and switchgrass – grow quickly. Some of the other biomass that would be used is waste product today, such as corn stover (the leaves and stalks left in a field after harvest), mixed hardwood left over from lumber operations, or even limbs left in the forest by timber cutters. The coals being evaluated include Illinois #6, Wyodak, Pittsburgh River Basin, North Dakota Lignite and Texas Sub-bituminous.

Other biomasses used in the NETL research are distillers’ dried grains with corn fiber, and algae produced for biomass in algae farms.

Even though there’s no question that co-gasification can produce a very flexible product stream, there are uncertainties that are being addressed by the NETL research.

“There are technologies to gasify coal and to gasify biomass, but there are uncertainties on how to mix them,” Morreale explains. For instance, how does the quality of the feedstock affect the quality of the product? What are the optimum percentages of various blends of coal and biomass?

Geographic implications also must be addressed. NETL research is looking at how best to couple the coals and biomasses that make sense geographically. A specific type of coal in a location might be paired with a biomass at that location, thereby eliminating the need to transport the material.

As is true with most emerging technologies, one of the drivers to commercial utilization is economics. As energy prices increase, alternative approaches such as co-gasification become more attractive. NETL’s co-gasification research program for DOE’s Office of Fossil Energy has been going on for about a year. NETL researchers are using a small-scale gasification system to evaluate various products.

“The co-gasification technology is drawing lots of attention,” Morreale says. “NETL is the right place to be doing this type of research because of our expertise and many years of experience in doing research and developing technologies to address national energy needs. With this research, we’re trying to address industry’s concerns about co-gasification.”

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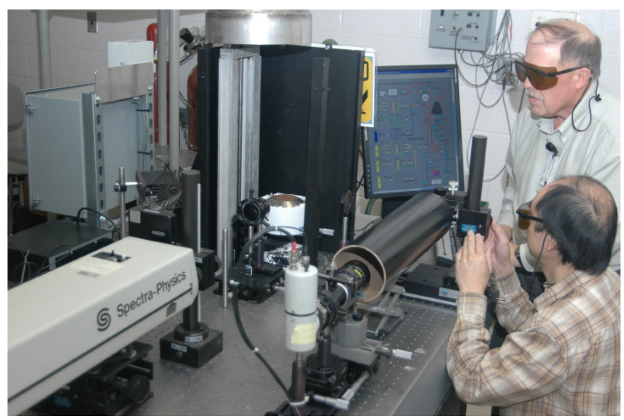

NETL researchers Joe Yip, seated, and Kent Casleton prepare an experiment in NETL’s unique test facility that enables measurement of oxy-fuel flames.

Unique New Test Facility Measures Oxy-Fuel Flames

NETL is developing a unique test facility that will enable measurement of combustion characteristics of oxy-fuel flames.

Oxy-fuel combustion schemes are being considered as a mitigation strategy to more efficiently reach the goal of zero carbon dioxide emissions from combustion of fossil fuels. The major products of oxy-fuel combustion are carbon dioxide and water.

Carbon dioxide can be separated simply by cooling the combustion products to condense out the water, yielding a concentrated carbon dioxide stream for subsequent sequestration. Safety permitting has been completed for NETL's test facility.

The NETL oxy-fuel-steam apparatus has been designed to perform combustion tests using flames with high steam levels representative of oxy-fuel systems.

The apparatus will be used for measurements of flame speeds and radiative properties of these flames, which are needed to accurately simulate and design advanced power systems for carbon sequestration. Shakedown operations are commencing.

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NETL Researchers Develop Procedures To Obtain Core Samples from Friable Coal

At many sites the nature of core samples, such as samples from the CONSOL sequestration project in Marshall County, WV, has made it virtually impossible to conduct necessary geomechanical measurements. The minerals are easily crumbled or pulverized making it very difficult to obtain useable core samples from potential carbon dioxide storage sites. The geomechanical properties of potential carbon dioxide storage sites must be determined before sequestration can be implemented.

Because traditional coring procedures had failed at the CONSOL site, NETL researchers developed another approach to obtaining useable core samples. They worked with a commercial water jet cutting company to adjust procedures to achieve successful coring of the larger samples. Several coal seam (Upper Freeport) and cap rock shale cores were prepared using this method. NETL is now in the process of installing its own water jet cutter.

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High-Speed Imaging Used to Study Particle Dynamics in Energy Processes

A new, high-speed digital imaging system, called High Speed Particle Image Velocimetry is being developed by NETL researchers to observe and measure the motion of small particles in energy processes. The imaging system reveals new details about the physics of particle interactions that have not been observed before. The system uses an endoscope similar to that used in surgeries to probe into particle flow fields and uses advanced imaging technologies from the high-definition TV industry. The new information about particle dynamics is being built into computer models for use in designing better fossil fuel power plants.

In many fossil fuel energy processes, fuels and catalysts are used in the form of small particles for solids transport and to enhance reaction rates. For example, in Integrated Gasification Combined Cycle (IGCC) systems coal is gasified after being ground into small particles for use in entrained flow or fluidized bed gasifiers. These gasifiers and downstream equipment can include other dense particle flows for thermal management or gas cleanup. Understanding and modeling the motion and mixing of small particles with reactant gases are critical to improving the efficiency and reliability of advanced fossil fuel energy systems. The new imaging system also can be applied to other industries where particle dynamics are of critical importance, including the pharmaceutical, petrochemical, and food industries.

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NETL researcher Rich Pineault installing a fuel cell at the PSDF Wilsonville, AL. (Photo courtesy of Southern Company.)

NETL Completes Initial Testing of Fuel Cell Module at Wilsonville PSDF Facility

NETL completed installation and shakedown testing of the Multi-Cell Array (MCA) test skid at the Power Systems Development Facility (PSDF) at Wilsonville, AL. The array is a mobile platform developed to enable testing of solid oxide fuel cells on coal synthesis gas.

The unit is designed to enable testing for up to 12 individual fuel cells over a range of electric load conditions for extended periods of time to provide data on the influence of trace coal contaminants such as arsenic, phosphorous, selenium and mercury on performance of fuel cells operated on coal syngas. These data are critical for development of fuel cells for coal-based power generation.

Shakedown testing on hydrogen for over 100 hours showed good results on five of 12 cells, and identified a need to improve sealing. Cell voltages were close to open circuit voltage and were stable over the test period.

Although the goal of testing on coal syngas was not met during the previous PSDF run due to interruptions in gasification operations, the NETL research team established a great working relationship with the operations team at Wilsonville. Results of the shakedown testing that was completed will lead to significant improvements prior to the next gasifier run at the PSDF facility. Modifications to the seal method are underway so as to achieve 100% cell operation before the next gasifier run which is scheduled for sometime this summer.

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Carbon Dioxide Storage Capacity Estimates for Coal Discrepancies Explained

A study by NETL researchers confirmed that pulverized coal powder samples can be used to estimate coal sorption capacity at relatively low CO_2 pressure. CO_2 sorption measurements on crushed and pulverized coal powder can be misleading if used for prediction of the CO_2 transport and sequestration in coal seams as they do not account for differences in texture and porosity.

Researchers compared the storage capacity of the dry Upper Freeport coal powder and lumps in a 9-month-long study. The pressure equilibration time was about one week at each pressure step to eliminate effects of the differences in diffusion rates and the accessibility of the micro-pores. While the study confirmed that the powder samples can be used to estimate sorption capacity at low pressure, sequestration is likely to involve the use of high pressure (supercritical) CO_2. At these pressures, observed differences in the magnitude of the sorption mechanisms, such as enhanced capillary condensation, with or without subsequent dissolution, demonstrate the importance of the changes in mesoporous texture caused by grinding of coal lumps into powder. The low-pressure Langmuir parameters suggest that the micropore system (matrix) differences between the powder and lumps are less dramatic.

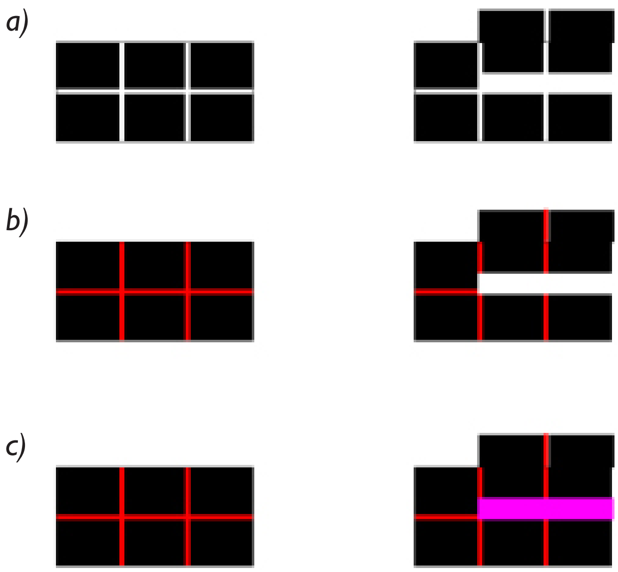

Illustration of the differences in CO_2 sorption on coal lumps (left) vs. powder (right): a) changes in mesoporous structure of the building blocks caused by coal grinding; b) low-pressure adsorption in micropores (red); c) high-pressure sorption (two mechanisms).

The results of the study were reported in an article by Vyacheslav Romanov and Yee Soong entitled, "Long-Term CO_2 Sorption on Upper Freeport Coal Powder and Lumps," which was recently published in *Energy & Fuels 2008.* Click here for link to article.

Contact: Yee Soong, 412-386-4962, and Vyacheslav Romanov, 412-386-5476

NETL Participates in *Materials Research Society Bulletin* Special Issue

NETL researchers recently contributed to a special issue of the Materials Research Society Bulletin on harnessing materials for energy. The issue focuses on the major global issues associated with energy conversion. The MRS Bulletin special issue, published in April, has contributions from energy experts from numerous countries, and reflects not only the growing global concerns about energy but also the opportunities that materials researchers can address in managing energy resources, storage, transformation, and efficient use. Specifically, the article authored by Drs. Cindy Powell and Bryan Morreale of NETL, "Materials Challenges in Advanced Coal Conversion Technologies," detailed the materials issues and current research areas associated with the conversion of coal to hydrogen, electricity and liquid chemicals, while mitigating greenhouse gas emissions.

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MFIX Multiphase Code Improved to Represent Complex Geometries

The multiphase computational fluid dynamics code MFIX (Multiphase Flow with Interphase eXchanges) developed at NETL is being updated to handle curved and inclined boundaries. Currently, the discretization is performed on a Cartesian (rectangular) grid system. Complex geometries with curved or oblique boundaries are approximated by a series of staircase steps. As a result, a very fine grid is required to accurately resolve pressure and velocity gradients near the walls. A new "cut-cell" technique is being implemented to represent curved boundaries and sloping walls. The computational cells are truncated at the wall to conform to the shape of the boundaries. Preliminary results

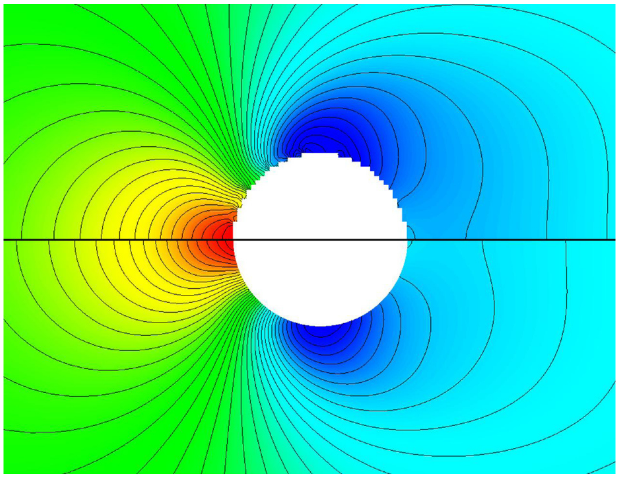

Figure 1. Pressure contours for the flow around a cylinder. Top: Staircase step method, bottom: Cut-cell method.

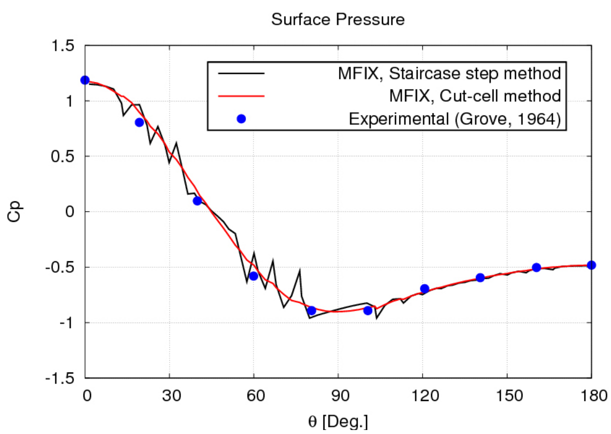

Figure 2. Surface pressure distribution along the cylinder.

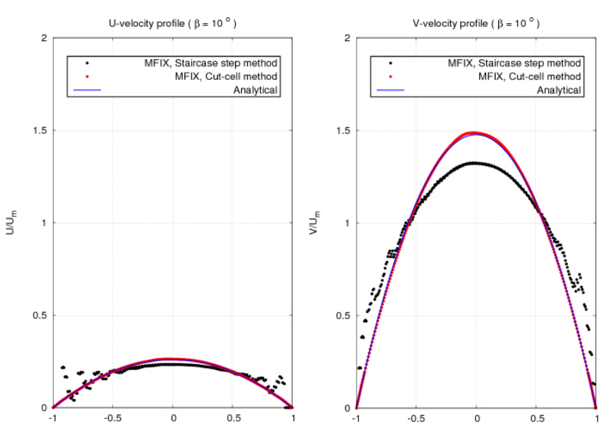

Figure 3. Velocity profiles in a skewed channel.

obtained with the new cut-cell technique show a clear improvement over the usual staircase step method, for the single-phase two-dimensional flow within an inclined channel. Velocity profiles are in excellent agreement with the analytical solution. Additional efforts are underway to extend the cut-cell method to three-dimensional multiphase flow. When completed, the enhanced version of MFIX will have the capability to represent complex geometries accurately.

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NETL Presents Carbon Capture Technology at AFS Annual Conference

Abbie Layne, a division director in our Office of Research and Development, served as an invited panelist at the 2008 American Filtration Society Annual Conference held in King of Prussia, PA on May 19-22. She presented an overview of NETL's Technology Transfer Program and an update of a novel technology for carbon capture, the supported ionic liquid membrane. NETL is developing the membrane for capture of carbon dioxide from gasification coal-fired power plants.

Membranes have already demonstrated the capability to separate hydrogen and carbon dioxide in various applications and types of systems but must overcome elevated temperatures and pressures as well as degradation by contaminant gases and particulates. In a joint project, researchers at the University of Notre Dame synthesized and characterized ionic liquids, while researchers at NETL incorporated candidate ionic liquids into supports, then evaluated the membrane performance for the resulting materials. The AFS requested this presentation as an example of advanced technology ready for technology transfer to a commercialization partner.

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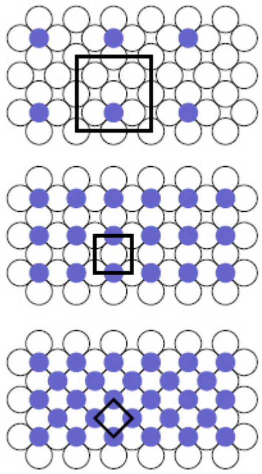

Models for mercury adsorption on face centered cubic metal surfaces. Open circles represent substrate atoms and filled circles represent adsorbed mercury atoms. (in fourfold hollow positions.)

NETL Paper Describes Interaction Properties of Mercury with a Series of Metallic Surfaces

A paper by NETL scientist Jan Steckel describing density functional theory calculations modeling mercury adsorption on metal surfaces has been published in *Physical Review B*. Density Functional Theory (DFT) calculations were used to elucidate fundamental information about mercury interaction with a series of metal surfaces that may be incorporated in novel mercury oxidation or sorbent technologies.

Mercury in the flue gas from coal-fired power plants represents a significant pollution problem in the United States. Because oxidized mercury is removed more readily from flue gas than elemental mercury, there is a need for effective and regenerable mercury oxidation catalyst materials. In addition to their incorporation into possible oxidation catalyst materials, noble metals including palladium, copper, silver, and gold also have been considered for inclusion in mercury removal sorbents, not only in the context of conventional power plants but within the context of integrated gasification combined-cycle power generation plants.

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Researchers Verify NETL Mercury Sorbent Mechanism

Researchers at the University of Cincinnati have verified a mechanism, first proposed by researchers in our Office of Research and Development, for sorbent capture of mercury by multivalent metal oxide sorbents. Lattice oxygen from a manganese oxide sorbent on a titanium oxide support was experimentally shown to capture elemental mercury from simulated flue gases. The NETL sorbent work, and proposed mechanism for sorbent capture, was extensively cited by the Cincinnati group in a paper published in the American Chemical Society journal *Energy & Fuels*. The Cincinnati researchers also successfully combined low temperature mercury capture and de-NO_x capabilities using the same titanium oxide supported manganese oxide material. The poisoning of the sorbent-catalyst by sulfur dioxide, first predicted by NETL researchers, was also observed.

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AAPG Hedberg Series Volume 3 Includes Paper on Tight Gas Resource Assessments

A paper by NETL's Ray Boswell and Kelly Rose has been published as part of the May 2008 American Association of Petroleum Geologists' Hedberg results volume, "Understanding, Exploring, and Developing Tight-gas Sands." The paper was part of Boswell and Rose's 2001-2005 work on NETL/DOE's tight gas resource assessments of the Anadarko, Greater Green River, Uinta, and Wind River basins. In 2005 Boswell and Rose presented and participated in the AAPG's Hedberg Conference, which was convened to gain a better understanding of tight-gas sand resources through presentations by and discussion among leading scientific and engineering experts.

The results of the conference led to improved exploration models and development and completion strategies required to exploit the vast North American tight-gas sand potential and emerging international tight-gas sand plays. Following the conference Boswell and Rose wrote their paper titled "Characterizations and Estimates of Ultimate Recoverability for Regional Gas Accumulations in the Greater Green River and Wind River Basins."

These assessments continue to garner interest from industry, including a request this month from geologists at Shell Exploration Inc. for a copy of the results CD for the Uinta basin assessment. To date, over 1000 copies of the results CDs and data DVDs for these studies have been distributed to researchers and industry.

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Collaborators Achieve Electrochemical Separation Proof-of-Concept

Researchers from NETL and Carnegie Mellon University, collaborating through the University Research Initiative, have assembled and operated a low-temperature electrochemical cell. High-temperature molten carbonate electrochemical cells have been shown to separate carbon dioxide (CO_2) from flue gas streams produced by pulverized coal combustion for power generation. However, the presence of trace contaminants, such as sulfur dioxide and nitric oxides, will impact the electrolyte within the cell. A lower temperature cell could utilize the benefits of commercially-available, upstream desulfurization and denitrification in the power plant to enable the CO_2 separation technique and make carbon sequestration more viable.

In the proof-of-concept testing by NETL and CMU researchers, an anion exchange membrane was sandwiched between gas diffusion electrodes consisting of a nickel-based electrocatalyst on carbon paper. When a potential was applied across the cell and a mixture of oxygen and carbon dioxide was flowed over the wetted electrolyte on the cathode side, a stream of CO_2 to O_2 of about 4:1 was produced on the anode side, suggesting that bicarbonate ions are the CO_2 carrier in the membrane. Although a mixture of CO_2 and O_2 is produced, the possibility exists to use this stream in oxy-firing of additional fuel. The results from the proof-of-concept electrochemical cell tests are encouraging and further optimization of the cell regarding material and energy requirements is warranted.

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ASME Publishes NETL Gas Turbine Fuel Cell Hybrid Research

NETL research on coal-fired gas turbine fuel cell hybrid power generation systems with CO_2 capture was presented at the Fuel Cell Science and Engineering Conference in Denver, CO, on June 16. The paper compared two different system configurations, recuperated and non-recuperated, both of which employ a unique carbon capture technology using an isolated anode stream for the fuel cell. In each case the calculation results show how efficiency gains can be made by increasing the system pressure ratio. The calculation results also show future direction to take in the configuration design of high-efficiency gas turbine fuel cell hybrid power generation systems. The paper was written by John VanOsdol, Randy Gemmen and Eric Liese. The work will be published in the conference proceedings and also will be published in the *Journal of Fuel Cell Science*.

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