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netlog

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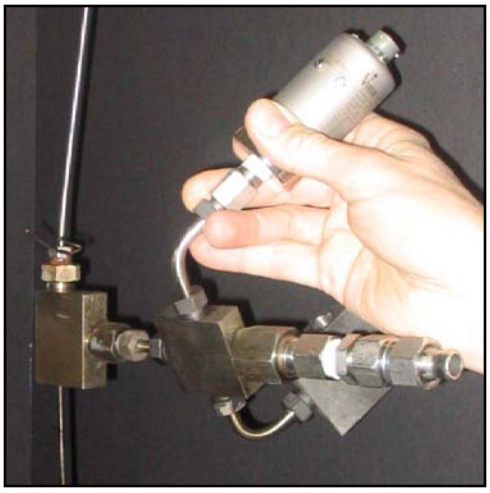

Microreactor Developed for Accelerated Testing of Fuel Thermal Stability

- NETL researchers on the Defense Fuels
- Team have designed, constructed, and
- begun operation of a microreactor
- that will enable testing of the thermal
- stability of liquid fuel formulations.
- This research is in support of the
- Department of Defense's long-range
- initiative to develop a single, fully-
- synthetic hydrogen-rich fuel capable of
- powering fuel cells as well as ground
- vehicles, aircraft, and ships. In order
- for the fuel to meet the performance
- specifications of the end-use equipment,
- certain additives will be required.
- NETL is attempting to identify the
- best additives that will allow the fuel
- to meet equipment specifications
- and Department of Defense needs.
- During this process it is important
- that the additive not impart negative
- properties to the fuel, such as degrading
- its thermal stability.

- The new microreactor will allow
- researchers to test fuels under
- conditions that mimic those that they encounter over longer periods of time in advanced military aircraft fuel systems. Subsequent analysis of the fuel composition to identify products of oxidation will help to determine the ability of the additive-containing fuel to withstand the effects of thermal stress. NETL researchers are currently screening the effects of potential seal-swelling additives on the stability of a synthetic JP-5 jet fuel. Initial results were presented at the Alternative Energy NOW Conference in February 2007, with additional information to be presented at the 10th International Conference on Stability, Handling, and Use of Liquid Fuels in the Fall of 2007.

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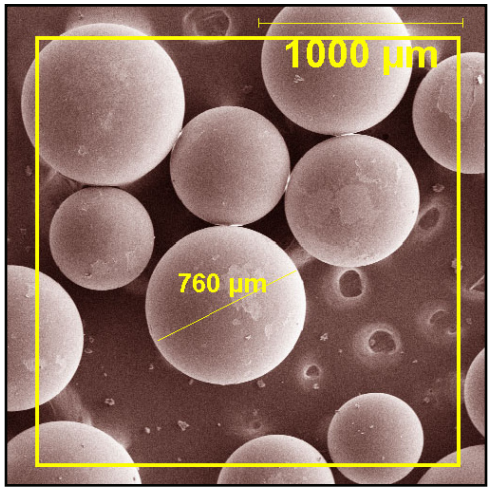


Poly Methyl Methyl Acrylate Sorbent

NETL Joins Forces with Medical School to Develop Sorbents

Researchers from NETL, West Virginia University's School of Medicine, and the University of Pittsburgh's Chemical and Petroleum Engineering

Department are working on a project to produce sorbents. They're applying a nanotechnology that is being used to create medical implants that won't cause infection and to prepare microcapsules for drug delivery. The project, which is part of NETL's University Research Initiative, is determining if a process called electrostatic layer-by-layer self-assembly (LBL) can be used to produce a better sorbent to remove carbon dioxide from fossil energy combustion gases. It is regarded as the most promising method to prepare multilayer nanocoatings of controlled thickness and composition.

The research project is aimed at using LBL to apply a uniform deposition of amines onto substrates to produce more effective sorbents. LBL is used to treat surfaces of medical implants to prevent infections in patients, or to deliver precise doses of medicine. The research builds on the complementary strengths of the three parties. NETL researchers are expert at developing solid sorbents for fossil energy applications. The WVU researcher has nanotechnology and bioengineering expertise to apply chemicals to different surfaces. And the University of Pittsburgh researchers have expertise in reactor and process design, modeling, and scaleup. For additional information about this project, click here. An associated article appeared in All American Patriot,com on March 9, 2007.

Contact: McMahan Gray, 412-386-4826

The Multiphase Flow Research Group in the Office of Research and Development at the National Energy Technology Laboratory develops capabilities to accurately model fossil power generation technology employing dense, reacting multiphase flow. From left to right, Sofiane Benyahia, engineer; Madhava Syamlal, engineer; and Phillip Nicoletti, computer scientist, look at details of a visualization of a fluidized bed gasifier.

Project Launched to Boost Simulations to Near Teraflop Speed Using MFIX

NETL has started a project to improve the accuracy of the calculations done with MFIX (Multiphase Flow with Interphase eXchanges) software for coal gasifier simulations by increasing the speed of calculations. The targeted computational speed would amount to approximately a trillion calculations per second. MFIX is software being developed at NETL for modeling multiphase reactors in fossil fuel processing plants. The latest version of MFIX includes two major capability enhancements. One modification improves the discrete element model's accuracy and speed. The other enhancement allows engineers to model the particle size distribution typically found in gas-solids reactors. The twin challenges being addressed in the project are the efficient use of a large number of processors and the management of the large data files resulting from the calculations. The project was started with the encouragement of the DOE Under Secretary for Science.

Gasifier simulations currently achieve sustained speeds of 20-100 gigaflops on parallel computers. The objective of the current project is to achieve a speed close to one teraflop in gasifier simulations. A teraflop is a trillion floating point operations per second. The Office of Science funded 500,000 CPU hours on a CRAY XT3 machine at the National Center for Computational Sciences at Oak Ridge National Laboratory for the project.

Contact: Madhava Syamlal, 304-285-4685

NETL Scientists Asked to Produce Two New Alloy Systems for Army

NETL was asked to produce a minimum of two new alloy systems for the Army Research Laboratory's Armor Mechanics Branch. ARL has tried unsuccessfully to have these systems produced elsewhere. ARL officials said NETL's unique materials capabilities make it the only place where this work can be done. If the work is determined to be feasible, NETL will supply, on a cost-reimbursable basis, these alloy systems in the forms needed by the Army. These alloy systems are critical to the performance testing of new armor applications needed to protect soldiers and military systems now being fielded throughout the Army's areas of operations.

Contact: Paul C. Turner, 541-967-5863

Carl Bauer and Steve Zitney

NETL Wins Two Awards from Federal Laboratory Consortium

The Federal Laboratory Consortium for Technology Transfer has announced that NETL has won two prestigious awards in recognition of our technology transfer efforts. Carl Bauer was selected as a winner of the Laboratory Director of the Year Award. Mr. Bauer's selection is an honor that recognizes his efforts and the entire NETL technology transfer program. Steve Zitney in NETL's Office of Research and Development will accept an FLC Award for Excellence in Technology Transfer for our successful transfer of the APECS software package. The awards will be presented at the FLC National Meeting in Arlington, Texas, on May 17.

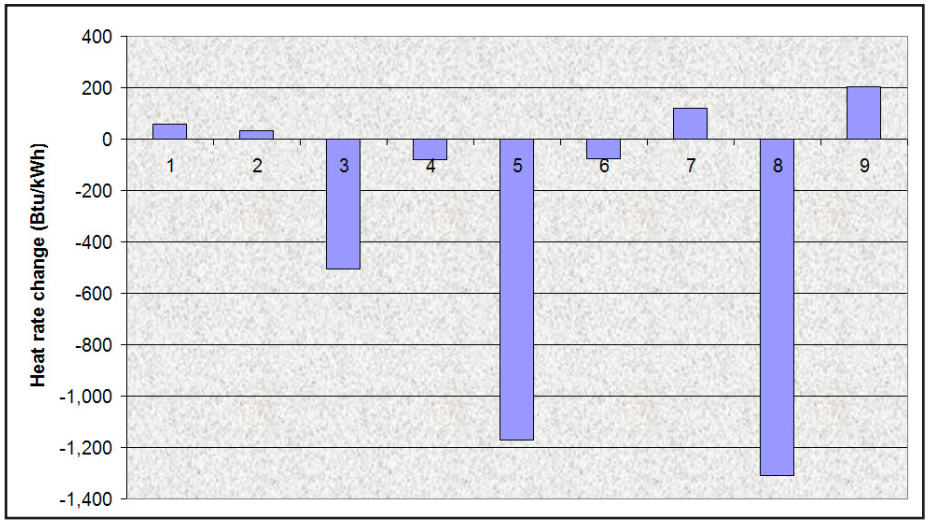
Contact: Diane Newlon, 304-285-4086

NETL Scientists Model Advanced Technologies for Oxy-Fuel Power Plants

Advanced oxy-fuel designs for greenfield applications are being developed by NETL researchers in cooperation with NETL's Office of Systems, Analysis, and Planning (OSAP). The technology changes that show greatest potential for improvement will be further examined by OSAP. Oxy-fuel combustion has significant potential for carbon dioxide capture, as it concentrates CO_2 in the off-gas stream from power plant boilers. Due to demand for subcritical plants, they are the initial focus.

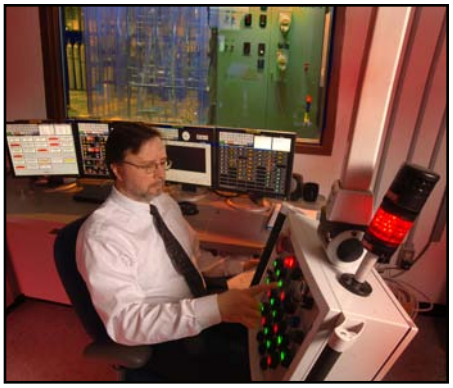
Modeling uses GE's GateCycle software, and takes the approach of designing a base plant, then identifying segments of the technology with the greatest potential for improving heat rate over the base case. Eight plant models were compared. The base case is an advanced boiler with inputs of coal, 95% pure oxygen, and recycling 45% of the total flue gas. Seven alternate configurations considered changes in oxygen purity, recycle rate, cooling of recycled gas, percent excess oxygen, and heat recovery.

Contact: Cathy Summers, 541-967-5844



Partial results of GateCycle© modeling study and effect on heat rate of changes to oxy-fuel combustion parameters. All options are compared to a new-design advanced technology green field sub-critical boiler. Parameter changes are:

1. Increased oxygen purity
2. No recycle of flue gas
3. Cooled recycled flue gas
4. Increased recycle rate
5. Cooled recycled gas at higher recycle rate
6. No heat recovery from compression
7. Reduced excess O2 fraction
8. Combined effect of negative changes



Randy Gemmen adjusts settings in the control room of NETL's Fuel Cell Test Facility.

Study Defines Cleanup Targets for Coal-SynGas-Fueled SOFCs

NETL scientists are studying the effects of trace species found in coal syngas on the performance and degradation of solid oxide fuel cells. Results from this work will help define gas cleaning and fuel cell material requirements for utilizing SOFCs in high-efficiency FutureGen plants. NETL recently completed tests investigating the effect of hydrogen chloride on the performance of SOFCs.

Cells were operated at 800 °C and 900 °C while being supplied syngas containing 20 ppm and 160 ppm HCl. Syngas compositions and HCl levels were selected to represent coal syngas from a gasifier using present-day cold-gas-cleanup technology. At these levels of HCl exposure, significant amounts of degradation occurred with 14-27% performance losses observed over an exposure time of 100 hours. Warm gas cleanup technology under development for future IGCC systems is anticipated to remove HCl to levels below 1 ppm. When extrapolated to the 1 ppm HCl level, NETL results suggest that HCl will not cause significant performance degradation.

Contact: Randy Gemmen, 304-285-4536

New Disposal Method Tested at NETL for Coalbed Natural Gas Produced Water

To address concerns of the Wyoming Department of Environmental Quality (WDEQ), NETL has been asked to determine if electromagnetic (EM) surveys could supply subsurface information for produced-water systems and possibly apply the information to various disposal options. The EM surveys could be a predictive tool to avoid areas of high saline content and also may prove effective in tracking any subsurface movement of saline waters that could cause environmental concern. If the utilization of EM surveys becomes an effective application to these types of geographic settings, it may open up large areas for disposal of produced water associated with methane extraction from coalbeds.

The Wyoming Oil and Gas Conservation Commission estimates that as of early 2007, only 10% of the recoverable coalbed natural gas (CBNG) in the Powder River Basin of Wyoming has been produced. One of the biggest challenges facing industry has been the large volumes of water in the coal seams that need to be disposed of in order to produce the natural gas. Several options of disposal have been reasonably successful, but may add significant additional overhead to the costs of production. In addition, the industry is being challenged through the Wyoming legal system about the need to beneficially use large portions of the produced water.

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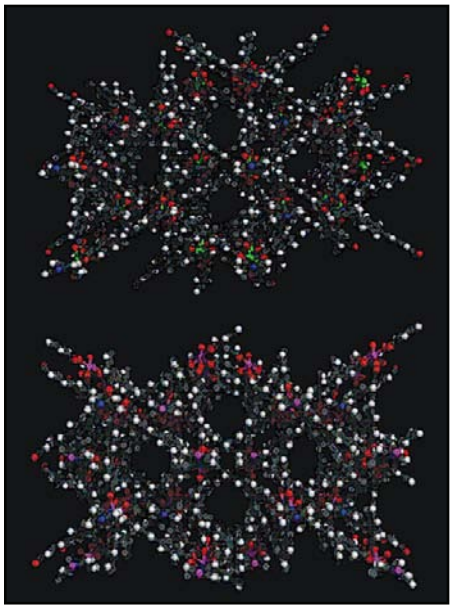

Molecular representation of new materials for separating clean hydrogen and carbon dioxide from gas.

New Method for Analyzing Adsorption Properties

A new method has been developed at NETL for the rapid assessment of the storage and transport properties of novel adsorbents. The new materials under investigation are intended for use in the capture or separation of carbon dioxide as well as organic vapors. A key parameter important to the evaluation of new adsorbents is the rate of transport of gases or vapors into and out of their pore system. The use of the new method to obtain this information is illustrated by a recent study of the kinetics of desorption of hexane from a metal organic framework. The metal organic framework was prepared by a collaborator at Rutgers University and features a microporous channel consisting of supercages connected by windows just large enough to allow passage of hexane.

The rates of hexane desorption were obtained using a pulse mass analyzer. The activation energy for this process was found to agree very well with the isosteric heat of adsorption measured by conventional methods. This new method will allow a rapid and accurate means to screen new adsorbents for their potential to separate or capture a wide variety of gases or volatile liquids. The results have been submitted in a paper to *Microporous and Mesoporous Materials*.

Contact: Bradley Bockrath
412-386-6081

NETL Scientists Developing Sensor Technology

NETL scientists presented progress toward the development of NETL's Vacuum Arc Remelting (VAR) sensors at a meeting of the Specialty Metals Processing Consortium (SMPC) on February 7 in Albuquerque. The SMPC is a not-for-profit consortium of specialty alloys and reactive metals producers. NETL has an agreement with the SMPC to produce a monitoring and diagnostic system for VAR melting to increase ingot quality. The technology, which is being developed by NETL scientists, utilizes the stray magnetic fields generated during operation of the VAR to estimate arc motion, which is an indication of the smoothness of the furnace run. The information provides an estimation of the quality of the ingot.

Gas turbine technology requires very high-quality superalloy ingots in order to produce the parts for the hot side of the turbine that meet the design requirements for service life. This includes critical, high-temperature rotating parts like turbine blades and buckets. By obtaining operational information relating to ingot quality, control systems can adjust the furnace performance on the fly to avoid conditions that lead to defects within the ingot. The technology has been lab tested on NETL's VARs.

Contact: Paul King, 541-967-5948

Evaluation Completed of Sulfur's Effect on Palladium-Based Membrane Reactors

NETL researchers have completed a series of experiments on the effect of sulfur on palladium-based membrane reactors that could improve the efficiency and reduce the cost of hydrogen production from coal. The identification and integration of membrane technologies into a gasification process has the potential of increasing efficiency, reducing capital costs and decreasing the production costs of hydrogen. The NETL experiments demonstrated the feasibility of the high-temperature water-gas shift in palladium and palladium-copper membrane reactors without added catalysts and in the presence of sulfur. The integration of a membrane separation device into the water-gas shift reaction has the potential of near-complete conversion of CO while producing a high-purity hydrogen stream and a high-pressure CO_2-enriched stream that can ultimately be sequestered or co-sequestered.

Contact: Charles E. Taylor,
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NETL Develops New Alloys for Use in Solid Oxide Fuel Cells

NETL has produced six new alloys for solid oxide fuel cell applications. NETL materials designers used a combination of computational approaches to design the alloys before producing them for testing. The predictions were used to optimize the development process of the oxidation-resistant alloys for service applications in the extreme environments found in solid oxide fuel cells. The six alloys are being tested to validate the estimates of their oxidation resistance.

The designers used the computational approach, first to estimate the as-produced phase stability and second to investigate the oxidation resistance through diffusion-controlled transformations. In the first case, steady-state thermodynamic modeling was utilized to predict the as-cast phases and to investigate the long-term effects of the phase stability under service temperatures. In the second case, the oxidation resistance was ranked by comparing the diffusivity of the protective species (e.g., chrome) with that of the base species (typically iron or nickel).

Contact: Paul Turner, 541-967-5863

NETL Researchers Make Progress in the Science of Gas Separations

NETL researchers have identified a promising new material as a potential agent for the separation of clean hydrogen and sequestration-ready carbon dioxide. The material is similar to the well-known inorganic dye, Prussian Blue. NETL researchers used sophisticated infrared spectroscopy to discover that this material adsorbs carbon dioxide instead of hydrogen. This study of the basic science of gas adsorption could be of use in gas separation applications. The results of the study have been released on the web prior to publication in the highly regarded scientific journal, *Journal of Physical Chemistry C*.

NETL researchers investigated various materials in their studies of gas separation properties. The adsorbents are Prussian Blue analogues that form in cubic crystals with the formula $M_3[CO(CN)_6]_2$. Vacancies within the crystal create micropores that can be filled with gas, leading to a high surface area. Hydrogen and carbon dioxide isotherms were obtained to correlate the amount of gas taken up with pressure. The isosteric heats of adsorption for hydrogen were about 6 kJ/mol, a relatively high value compared with those for similar adsorbents. For carbon dioxide the values were 25 kJ/mol, which reflect the larger interaction potential of this gas. The infrared study demonstrated that after the surface of the Prussian Blues had been saturated with carbon dioxide it required the addition of nearly a million-fold excess of hydrogen to displace the more firmly held gas.

Contact: Bradley Bockrath, 412-386-6081

Mineral Additive Improves Character of Well-Plugging Cement

NETL tests of the curing of four oil-well-plugging cements in a supercritical CO_2 environment indicate that one CO_2-reactive mineral additive significantly improves cement performance, based on physical and chemical characteristics. Safe storage of CO_2 in depleted oilfields and/or saline aquifers depends on the integrity of cements used to seal legacy and CO_2 injection wells.

Four cements (one unmodified and three containing 20% of different CO_2 reactive mineral additives) were cured under laboratory conditions simulating the pressures, temperatures, and chemistry of a saline aquifer; supercritical CO_2 was maintained in contact with the cements throughout the tests. All cement cores developed an altered zone of calcium carbonate; the altered zone of a 100% cement core constituted 45% of the total core, while a cement core containing 20% of one of the mineral additives had an altered zone that accounted for just 7% of the total mass of core.

Contact: Paul Turner, 541-967-5863

NETL Researchers Continue Collaborative Work on Field Project for Coal Seam Sequestration

NETL researchers met at the CONSOL research center with West Virginia University researchers and CONSOL personnel to continue planning and data evaluation for the DOE cofunded coal seam sequestration field project in Marshall County, WV. Geologic data from the field project and from the West Virginia Geologic Survey have been collected and are being used to construct a geologic model for input to planned reservoir engineering simulations. Proposals for well logging, coring, and well-test operations are being developed. These additional data will be needed for the geologic and engineering modeling. Plans for a variety of joint NETL-WVU-CONSOL environmental studies also were discussed.

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

Patent Granted on Flow Control Device for Fuel Cells

NETL has been granted a patent on a Micro Electro Mechanical System (MEMS) device that can control small amounts of flow. The device was invented as a means to improve flow distributions within fuel cells, although other applications such as flow control in combustion systems for NOx control are possible. NETL researchers in the Office of Research and Development share the patent with two faculty members from the University of Pittsburgh. NETL continues to collaborate with the university on development of sensor and control technology for energy applications through NETL's University Research Initiative Program

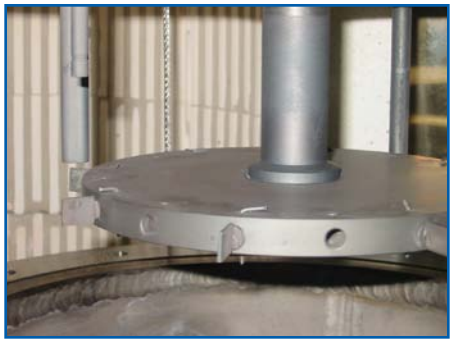
Contact: Randy Gemmen, 304-285-4536

NETL Researchers Develop Method for Measuring Sorption Isotherms and Diffusion Rates in Coal for Carbon Dioxide Sequestration

NETL researchers have invented and successfully tested a new method for simultaneously measuring isotherms and diffusion rates for carbon dioxide sequestration in coal seams. Compared to other methods for non-powdered samples, NETL's ambient-pressure gravimetry is simple, direct, and inexpensive. A paper that describes this invention has been accepted for the International Coalbed Methane Symposium, Tuscaloosa, Alabama, May 25-27. 2007.

Sorption isotherms and diffusion rates are needed as inputs for reservoir engineering computations of sequestration capacities and field-project designs. Sorption isotherms are conventionally measured on powdered coal by a pressure-drop (i.e., manometric) method. However, it is difficult to obtain diffusion rates from this experimental technique, and powdered samples may give unrealistic sorption capacities. In the ambient-pressure gravimetric technique, larger (centimeter-sized) pieces of coal are weighed and then exposed to carbon dioxide (or other gas) for the desired pressure, temperature, and sorption time. The high-pressure cell then is quickly depressurized, and the sample weight is automatically recorded on a conventional laboratory balance at fixed time intervals for a period of about one hour. A plot of sample weight vs. square-root of time yields a straight line. The rate of diffusion can be obtained from the slope of the line; the difference between the intercept of the line and the weight of the sample before exposure to the gas gives the amount of gas sorbed by the sample.

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



The Hostile Atmosphere Elevated Temperature Erosion test is used to study erosion and corrosion in a gas environment.

Pratt-Whitney Rocketdyne Collaboration to Assess Wear Performance of Alloys for Gasification Industry

Utilizing NETL's unique wear-testing capabilities, scientists will shortly begin assessing the tribological performance of a suite of potential structural materials in collaboration with Pratt-Whitney Rocketdyne of Canoga Park, California. NETL will determine the relative stability of these materials in environments that include elevated temperatures, as well as exposure to erosive particulate and corrosive gases.

The studies will utilize the Hostile Atmosphere Erosion Test (HAET) developed by NETL. The HAET, designed to simulate the effects of wear-corrosion synergies that can develop at high temperatures in service environments that are typical of gasification and combustion processes, is part of the Severe Environment Corrosion and Erosion Research Facility (SECERF) at the Albany site.

Contact: Joe Tylczak, 541-967-5849

University Collaboration on CO_2 Capture Initiated

Researchers from West Virginia University, the University of Pittsburgh, and NETL convened at NETL to initiate research on a recent collaboration through the University Research Initiative. The research will establish the feasibility of developing low-cost, highly-efficient, multi-functional solid sorbents for CO_2 capture using a novel nanotechnology. Researchers also will conceptually design a dry, regenerable sorbent scheme that uses a CO_2-capture sorbent. To achieve these requirements, the team of researchers was assembled to address basic and applied scientific and technological issues regarding sorbent development and reactor design. Rapid transfer of information among participants was established at the meeting and will be one action that promotes success in this research project.

Proposed methods for removing carbon dioxide from flue gas, for example monoethanolamine (MEA) scrubbing, suffer from several drawbacks including high parasitic power costs. Sorbents offer the potential to decrease the amount of energy required in the overall capture process, especially by increasing the carbon loading of a sorbent. The proposed nanotechnology provides a novel approach for grafting substantially larger amounts of the active component–amine in this case–onto the solid substrate as compared to currently studied sorbents. The sorbent will be used in a CO_2-capture system that requires an absorber coupled with a regenerator. This reactor scheme will be investigated in another part of the collaboration. The initial scheme will involve a fluidized bed for CO_2 absorption followed by a moving bed for solid sorbent regeneration. Chemical, physical, and transport properties of the sorbent will dictate the likelihood for use of this first reactor scheme and could lead to some changes in the conceptual design. Ideally, the capture scheme will use less energy compared with traditional MEA scrubbing, will be able to manage heat, and will minimize attrition losses.

Contact: Henry Pennline, 412-386-6013

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.