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ON THE COVER

NETL's computer simulation of a plantwide IGCC Process Dynamic Simulator Research and Training Center.

> netlog is a quarterly newsletter, which highlights recent achievements and ongoing research at NETL. Any comments or suggestions, please ct Paula Turner at paula.turner@netl.doe.gov or call

NETL's IGCC Dynamic Simulator Project Presented at Gasification Conference

Recent progress and future plans for NETL's Integrated Gasification Combined Cycle (IGCC) Dynamic Simulator Research and Training (DSR&T) Center project were highlighted at the 2008 Gasification Technologies Conference in Washington D.C. The presentation provided an overview of the collaborative, multi-year, multi-phase project, including a detailed update on the recently completed functional specification for a high-fidelity, full-scope, real-time, dynamic simulator for an IGCC plant with carbon capture. The presentation concluded with a discussion of future plans, schedule, and milestones for simulator development, testing, and deployment at the IGCCDSR&T Center.

The NETL IGCC dynamic simulator will combine, for the first time, a process/gasification dynamic model with CO₂ capture and a power/combinedcycle dynamic model together in a single dynamic simulation framework for use in engineering research studies, operability analysis, control strategy evaluation, and training applications. NETL has chosen to develop the simulator using software solutions provided by Invensys Process Systems (IPS). The integration of the dynamic models will be performed by IPS's SIM4ME technology which ensures the seamless, cyber-harmony necessary to provide all the functionality and performance required for real-time training applications. The best-in-class DYNSIM and InTouch software from IPS will be used to develop the dynamic simulation and human-machine interfaces, respectively.

NETL will use the simulator to establish a world-class IGCC DSR&T Center under the auspices of NETL's Collaboratory for Process & Dynamic Systems Research. The DSR&T Center will be co-located at NETL and the National Research Center for Coal and Energy at West Virginia University. Headquartered in Dallas, Texas, IPS is a major global supplier of systems, software, services and instruments for industrial process automation and asset performance management. The Gasification Technologies Conference is an annual worldwide gathering of the gasification sector of the energy industry.

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NETL Completes First Fuel Cell Exposure Tests Using Benzene Doped Syngas

Engineers at NETL are conducting tests to determine the effects of coal syngas trace species on the performance and degradation of anode-supported solid oxide fuel cells (SOFC). An exposure test of 500 hours was recently completed using coal syngas mixtures doped with 150 ppm of benzene. Higher hydrocarbons including benzene and naphthalene may deposit carbon within the anode electrode, thereby degrading cell performance. Benzene testing at 150 ppm exposure showed cell performance degradation at a rate of 6.6 percent per 1000 hours of operation.

This research is part of a continuing effort to examine the effects of minor and trace coal syngas species on SOFC performance. The results of this work will be used to identify acceptable contaminant levels for SOFC operation and will help define design targets for coal syngas cleanup systems. Additional tests will be performed in the coming months to evaluate other trace hydrocarbon species such as napthalene.

Contact: Randy Gemmen, 304-285-4536



West Virginia University graduate student Greg Hackett operates an impedance analyzer in support of NETL's fuel cell performance testing program.

NETL Researcher Presents Talk on Mercury Control Options

Evan Granite presented an invited talk on mercury capture from flue gas to the American Filtration & Separation Society Annual Fall Conference held in Charlotte, NC on September 25. In this talk, "Unmet Needs for Mercury Capture from Coal-Derived Flue Gas," Granite provided an overview of current and alternative technologies for mercury capture from coal-derived flue gas. He discussed five methods for mercury control and measurement within coalderived flue gas that have been recently developed at NETL, and highlighted future research needs for mercury control including improved sorbent-flue gas contact, development of poison-resistant sorbents and catalysts, new scrubber additives for retention of mercury within wet FGD systems, concrete-friendly activated carbons, new continuous measurement methods, and byproducts research.

With the USEPA's Clean Air Mercury Rule currently being reviewed by the Supreme Court, and many states promulgating their own regulations, the need exists for low-cost mercury removal techniques that can be applied to coal-burning power plants. The injection of powdered activated carbon into the ductwork upstream of the particulate control device is the most mature technology for mercury capture. Alternative techniques for mercury capture will also play a role in the near future because of the numerous configurations of air pollution control devices present within the power plants, as well as the many different coals being burned. These methods employ sorbents, catalysts, scrubber liquors, flue gas or coal additives, combustion modification, flue gas cooling, barrier discharges, and ultraviolet radiation for the removal of mercury from flue gas streams. The DOE Mercury Program has been a huge success, spurring development, demonstration, and commercialization of many technologies for the capture of mercury.

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



Novel carbon dioxide capture process inventors are, from left, Yee Soong, Sheila Hedges, and Robert Dilmore.

NETL Files for Patent on Novel Flue Gas CO₂ Capture Process

NETL has filed a patent application for a novel carbon dioxide capture process invented by NETL researchers. The process involves dissolving CO_2 into an aqueous solution and eventually separating it out. Preliminary calculations indicate that CO_2 could be separated by this process with as much as 20 percent less heat requirement than the typical monoethanolamine (MEA) scrubbing process. In the NETL process, the CO_2 from combustion flue gas dissolves into an aqueous solution of amine and soluble potassium carbonate. Potassium carbonate rapidly reacts with amine-associated carbamate and water to form less-soluble potassium bicarbonate that precipitates from solution.

This reaction serves both to chemically regenerate the amine solution by removing the carbamate and to separate CO₂ in the form of solid bicarbonate. Separated potassium bicarbonate can then be heated to regenerate back to solid potassium carbonate, releasing concentrated CO₂ gas. Finally, potassium carbonate is re-dissolved in the regenerated amine solution, and the reactive solution re-exposed to flue gas to close the process loop.

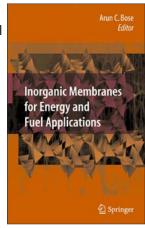
The process has the potential to achieve high CO₂ capture efficiency with relatively low regeneration energy requirements, suggesting that it could achieve CO₂ capture from utility emission streams at lower overall cost.

Contact: Yee Soong, 412-386-4925

Springer Publishes Book on Inorganic Membrane Materials and Processes edited by NETL Scientist

Dr. Arun Bose of the Strategic Center for Coal edited a new book entitled

"Inorganic Membranes for Energy and Environmental Applications." The study of inorganic membrane materials and processes is a rapidly expanding research area. Membrane-based technologies have the potential to improve the cost, efficiency, and environmental performances of energy production systems beyond current



benchmarks. This book documents progress in inorganic membranes, especially in advanced materials and novel separation concepts, with applications for cost-effective and environmentally progressive energy production solutions.

Membranes generically refer to a separation or coupled reaction-separation device. The chapter on "Progress in Ion Transport Membranes (ITM) for Gas Separation Applications," authored by NETL's Bose et al., presents the evolution and advances of ITMs for gas separation applications, especially for separating oxygen from air at much lower costs and higher efficiencies than conventional processes for standalone oxygen production plants and for integration of ITM Oxygen with advanced power production systems, such as IGCC.

The chapter on "Gasification and Associated Degradation Mechanisms Applicable to Dense Metal Hydrogen Membranes," authored by NETL's Morreale et al., discusses degradation mechanisms that dense metal hydrogen separation membranes may encounter in gasification environments. There are 17 chapters documenting the progress and applications of inorganic membranes to energy systems.

This book provides a good reference for researchers and research managers involved in inorganic membrane technology RD&D, for applications to future energy and fuel production systems and in addressing greenhouse gas emission concerns.

Contact: Arun Bose, 412-386-4417

Solvent Scrubbing System for CO₂ Capture Being Tested at Burger Station

A wet scrubbing technique for CO₂ capture invented at NETL and licensed to Powerspan Corporation is being investigated at the pilot-scale level at First Energy's Burger Station in Shadyside, Ohio. The ammonia-based scrubbing method has the potential to be placed on the flue gas streams from new or existing coal-fired power plants to produce a salable fertilizer and a pure stream of CO₂ that can be sequestered. This technology is being demonstrated at a 1-MWe scale.

The absorber and regenerator have been constructed and the mechanical commissioning of the system has been completed. Cycling of ammonia-based solution between reactors is occurring in this shakedown phase was completed in mid-December. Afterwards, a testing program will be implemented to establish a performance database using actual flue gas from the Burger Station.

Contact: Henry Pennline, 412-386-6013



NETL researchers open a manhole cover in front of historic John Wesley AME Zion Church in Pittsburgh, PA.

Geothermal Energy Technology Will Heat and Cool Oldest African-American Church

Three years ago, NETL researchers developed a concept for using geothermal energy from abandoned mines to heat and cool buildings with heat pumps.

Community leaders and local officials broke ground on October 31 to install a large heat pump that will use water from an abandoned mine to heat and cool the historic John Wesley AME Zion Church on Herron Avenue in Pittsburgh, the oldest African-American church still being actively used.

Many Pittsburgh buildings are plagued by runoff from abandoned mines, including the John Wesley church. Water runoff from a mine dating back to the 1800s seeped into the church basement. The Pennsylvania Department of Environmental Protection fixed the problem by installing a pipe on the mine floor that allowed the water to drain into the storm and sewage systems under the street. The church will now turn that water, which flows at a constant rate of 100 gallons a minute at 55 degrees, into an elegant solution to its energy needs.

The project is expected to cut heating costs by as much as 80 percent and cooling costs by 50 percent.

The concept of having heat pumps provide heating and cooling by using geothermal energy from water in underground mines was developed by NETL researchers in 2005 with funding provided by DOE's Office of Energy Efficiency and Renewable Energy.

A paper on the technology was published by the NETL researchers in the peer-reviewed journal *Mine Water and the Environment* in 2006. The researchers also helped the community group who are now using the technology to obtain funding from the state of Pennsylvania.

Recently, NETL has been monitoring the temperature of the mine water to demonstrate its constancy. The constant temperature is one of the reasons why this technology can potentially find applications elsewhere in mined areas. The approach being applied at the church is one that could be used at many sites in the region.

Contact: Bob Kleinmann, 412-386-6555

PSRI Asks NETL to Expand Collaboration on High Speed Particle Imaging System

NETL has developed a High Speed Particle Imaging technology that allows researchers to view and measure detailed behavior of individual particles in dense particle flows for the first time. Based on the success of initial tests, Particulate Science Research Inc. (PSRI) has asked to continue and expand its existing collaboration with NETL in an effort to apply NETL's technology to commercial industrial projects. PSRI is an industry-sponsored research organization funded by an international consortium of commercial companies.

PSRI does research on and troubleshoots commercial processes that use dense particle flow systems. NETL's research focuses on dense particle flows to better understand and improve the models (such as NETL's MFIX model) that are used to design and improve advanced power generation processes, including carbon capture and coal gasification.

PSRI asked NETL to apply the High Speed Particle Imaging technology to NETL sponsored research taking place in PSRI's labs in Chicago. The first tests of the High Speed Particle Imaging system provided new insight and encouraging results that produced detailed data regarding particle behavior critical to the NETL project. As a result of this collaboration, NETL is able to have its technology applied quickly to improve commercial projects in a wide range of companies.

Contact: Franklin Shaffer, 412-386-5964



SimVal combustor and team with the pressure vessel.

NETL Combustion Data Requested for CFD Model Validation

Researchers from NETL will provide data sets generated in NETL combustion test facilities for a new Small Business Innovative Research project focused on developing new computational tools for designing fuel flexible combustion systems. The goal of this project is to develop a turbulent combustion model for computational fluid dynamics (CFD) codes for use with hydrogen-fueled gas turbine combustors. A kickoff meeting for a Phase I SBIR project with CFD Research Corporation (CFDRC) was held November 21.

Diffusion effects are much more important for hydrogen than most other fuels, but turbulent combustion models typically don't account for these effects. By accounting for diffusion effects in a reduced order combustion model and validating these results against experimental data, the researchers at CFDRC seek to develop a practical, accurate, and computationally efficient tool that can be used in detailed simulations of fuel-flexible combustion systems. The CFDRC developers asked to use NETL combustion data for validating this simulation tool. The data sets provided by NETL will include data from NETL's Simulation-Validation Combustor which was designed and built to provide comprehensive data sets that can be used to develop and validate advanced combustion codes.

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Dr. Phuoc Tran Invited to Write Book Chapter on Laser Ignition

Dr. Phuoc Tran of the Environmental Science Division has been invited to write a chapter on laser ignition in the "Handbook on Combustion", edited by M. Lackner, F. Winter and A. Agarwal. The handbook will be published by VCH Wiley in 2009. It consists of five volumes including chapters contributed from 100 leading experts from industry and academia. The handbook will be a major reference work in its field, aimed at combustion researchers and engineers.

Use of a laser beam as an ignition source has many potential benefits over conventional ignition systems. With laser ignition, the control over ignition location, ignition timing, ignition energy and its deposition rate can be easily carried out. Also, laser ignition is nonintrusive, thus, heterogeneous effects and heat loss can be eliminated. It offers the opportunity for sudden release of specific radicals and the onset of specific reactions. This in turn may provide better means for controlling pollutant formation, ignition and flame stabilization especially for super-lean combustion applications. And above all, laser ignition is capable of providing center ignition and/or multiple ignition sites that can be programmed to ignite a combustible mixture, either sequentially or simultaneously, thereby facilitating leaner operations.

In addition, if a flame is initiated simultaneously at many points throughout the mixture volume, the total burning time could be much shorter than when using a single-site igniter. This could make laser ignition a potential technique for many practical applications such as gas reciprocating engines that operate with much higher compression ratios, faster compression rates, and much leaner fuel-to-air ratios. The laser ignition chapter, which will focus on the fundamental physics and practical applications of laser ignition, will appear in volume five of the handbook.

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Junwei Wu, a Ph.D. student at West Virginia University who is working with NETL's Office of Research and Development, displays the results from his electroplating research supporting long lifetime solid oxide fuel cells.

New, Improved Coating Process Developed for Solid Oxide Fuel Cells

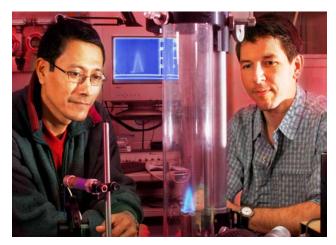
Manganese-cobalt coatings for solid oxide fuel cell (SOFC) interconnects have recently been developed as a result of a collaboration between NETL and West Virginia University.

The new process uses an electroplating technique that does not harm the environment. This electroplating process offers significant advantages in terms of cost and ease of operations over other coating methods.

Recent results during on-cell testing showed considerable improvement of SOFC degradation with this coating method as compared with uncoated interconnects. Further improvements are anticipated as optimized plating variables are identified.

The results of this research were presented at the Materials Science & Technology-2008 conference and were published in two peer-reviewed journals. An invention disclosure of the process has been filed as well.

Contact: Randy Gemmen, 304-285-4536



Dr. Don Ferguson, right, and a doctoral student from West Virginia University, were involved in studies of ways to update and improve methods of determining fuel interchangeability for various combustion applications.

Researcher Addresses Fuel Interchangeability at Washington Forum

An invited presentation was given by Don Ferguson of NETL to a number of gas producers, pipeline operators and their customers at the Platts Gas Interchangeability and Quality Forum held recently in Washington, DC. Dr. Ferguson discussed research underway at NETL to update and improve methods of determining fuel interchangeability for various combustion applications.

Fuel interchangeability continues to be a serious concern for pipeline operators and end users including power providers. The Energy Information Administration is predicting a substantial increase of imported liquefied natural gas (LNG) into the United States over the next 10 years. While LNG is similar in composition to domestic natural gas. the cryogenic process used to liquefy LNG results in higher percentages of heavier hydrocarbons in the fuel. This could potentially alter combustion properties in the end use applications, thus resulting in concerns regarding fuel interchangeability. Work at NETL, which is being funded through the Office of Energy Efficiency and Renewable Energy-Industrial Technologies Program, is focused on improving computational methods and related fundamental combustion characteristics to physical and chemical

properties of the fuels and burner geometries. This program initially looked at interchangeability issues between domestic natural gas and LNG, but has recently been expanded to include coal-derived syngas, landfill gas, biomass-derived gases and other opportunity fuels.

Contact: Don Ferguson, 304-285-4192

NETL and Sandia Join Forces on Rock Geomechanics Study

Researchers at NETL and Sandia National Laboratories plan joint research on rock geomechanics during FY 2009. Sandia will perform true tri-axial geomechanical and acoustic emission measurements on formation of shear and compaction bands in sandstone; NETL scientists will perform optical microscope, X-ray computer tomography, and other measurements on the rock specimens. NETL scientists also will use their model to interpret and predict the experimental behavior.

In the NETL model, fractures and shear bands begin as the breaking of the weakest cement bonds between sand grains, with the breakages distributed randomly throughout the rock sample. As the stress increases, more and more bonds are broken; but the appearance of newly broken bonds gradually becomes more concentrated in one region, resulting in the formation of a band or fracture. Fractures and compaction bands greatly affect the flow patterns of carbon dioxide, water, and other fluids through underground rock formations and thus can play major roles in geologic sequestration of carbon dioxide, or recovery of petroleum. However, because they are thin and usually vertically oriented, the presence of compaction bands is difficult to detect by means of either horizontal or vertical wells.

To initiate the planned research, an abstract by M. Ferer and Duane H. Smith, "Tracking the locations of failure events in a 2-D model," which describes the modeling work, has been submitted to the 2009 Conference on Experimental and Applied Mechanics of the Society for Experimental Mechanics, Albuquerque, NM, June 1-3, 2009.

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