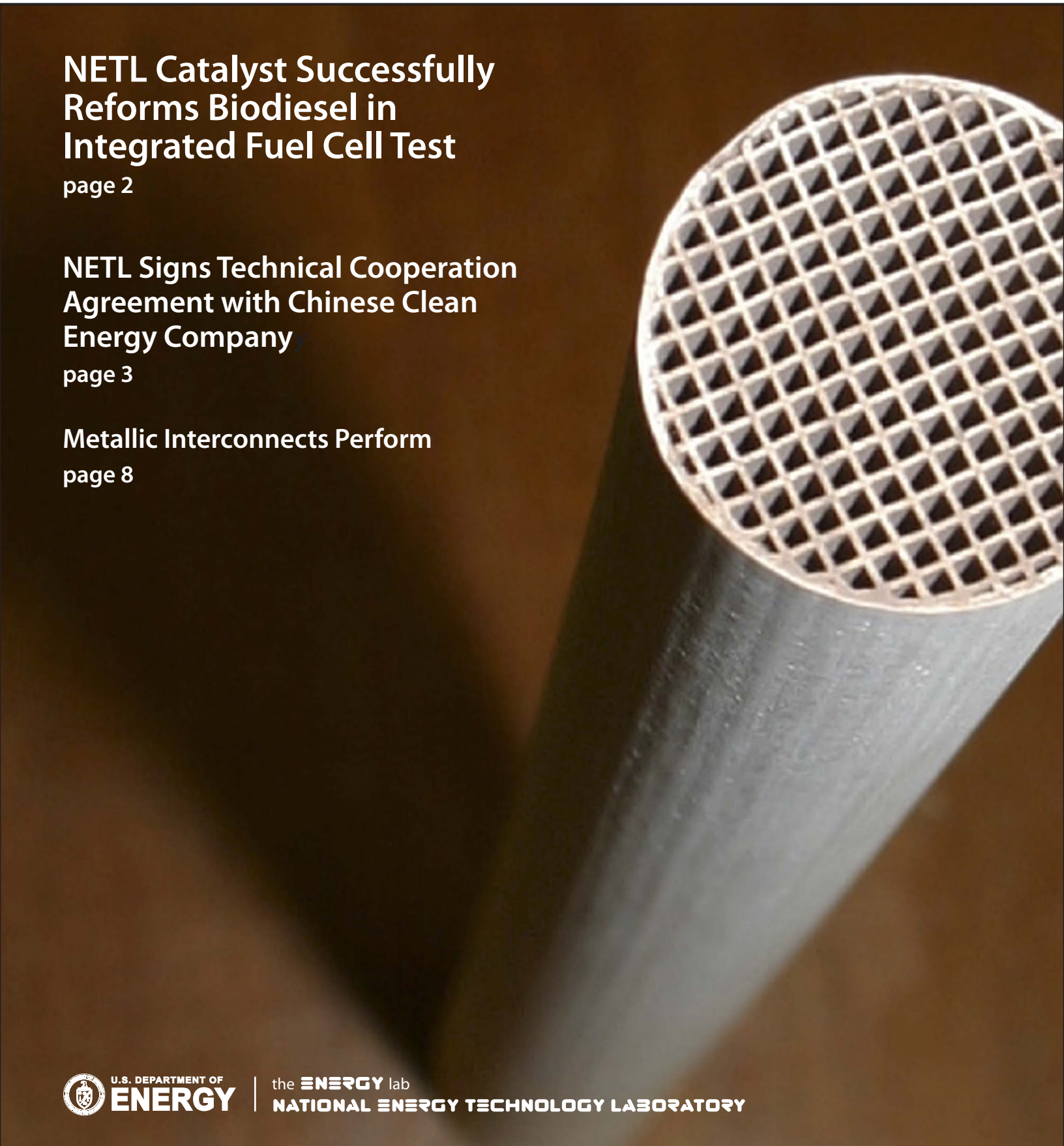
# netlognews

*NETL's R&D newsletter* *April 2010, Issue 17*





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NATIONAL ENERGY TECHNOLOGY LABORATORY

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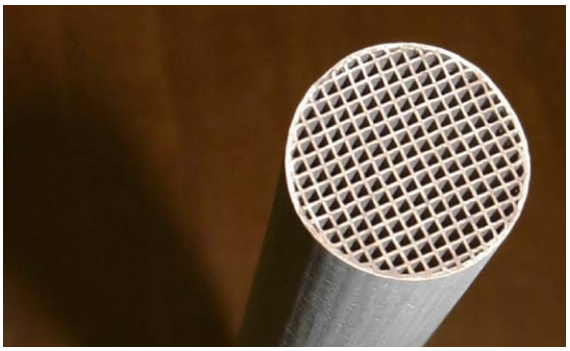
## ON THE COVER

*NETL Catalyst Successfully Reforms Biodiesel in Integrated Fuel Cell Test.*


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

*Diesel reforming catalyst.*

## NETL Catalyst Successfully Reforms Biodiesel in Integrated Fuel Cell Test

An NETL-developed catalyst exhibited stable, near-equilibrium performance while reforming biodiesel throughout a 100-hour test. Liquid biodiesel fuel reacting with air and steam across the monolithic structured pyrochlore-based catalyst produced hydrogen-rich synthesis gas that powered a fuel cell in the NETL Fuel Cell Test Facility.

Previously, more than 1,000 hours of continuous testing proved the catalyst successful in reforming commercial diesel, and more recently was reproduced and validated for reactor products at Precision Combustion Inc. (PCI), a leading developer and manufacturer of advanced catalytic reactor systems for aerospace, energy, transportation, chemical, and fossil fuel production industries. The amount of rhodium per kW of electricity produced—a major factor in determining the total cost of a reformer—was significantly less with the NETL catalyst than with others evaluated for the same PCI process.

Several more fuel cell developers, fuel reformers, and catalyst companies have expressed interest in evaluating the NETL catalyst for transforming diesel fuel quickly and reliably into clean syngas suitable for solid oxide fuel cell (SOFC) applications. This technology would help make SOFC-based auxiliary and/or distributed power units both practical and economical.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*Representatives from the ENN Group (China) and NETL officials gather to sign formal agreement for technical collaboration.*

## NETL Signs Technical Cooperation Agreement with Chinese Clean Energy Company

NETL officials and representatives from the ENN Group signed a 5-year Project Agreement for R&D cooperation developed under Annex IV (Energy & Environmental Control Technologies) of the U.S.--China Fossil Energy Cooperation Protocol led by ASFE James Markowsky for the United States. The signing follows meetings of senior ENN Group officials with DOE Secretary Stephen Chu, Under Secretary Kristina Johnston, Principal Assistant Secretary for Fossil Energy Dr. Victor Der, and NETL Acting Director Dr. Anthony Cugini. The ENN Group is a large, vertically-integrated Chinese energy supplier that is developing zero emission coal-based power, carbon capture, and renewable energy technologies.

The U.S.--China Clean Energy Research Center, jointly announced in November 2009, focuses on diplomatic and commercial initiatives on energy and the environment. The agreement aims to advance clean coal technologies of interest to both countries through collaborative R&D, modeling and simulation, researcher exchanges, joint publications, and other appropriate activities.

Contacts: Margaret Lou, 281-494-2514 and Scott Smouse 412-386-5725

*UNEP/GRID Arendal international steering committee at work.*

## U.N. Environmental Program Review of Gas Hydrates R&D

The United Nations Environmental Program (UNEP/GRID-Arendal) kicked off its global review of methane gas hydrates in the natural environment with a meeting of its international steering committee on March 4 and 5 in Arendal, Norway. Steering committee members, including two researchers from NETL as well as leading researchers from Canada, Japan, Germany, Korea, India, and Norway, worked for two days to finalize the outline and goals for the project, which will ultimately result in the publication of a hard copy book, e-book, and web-based information portal. These references will provide interested parties with basic information about gas hydrates and their role in the natural environment. They will also discuss global climate cycle and energy security implications of naturally occurring gas hydrates as well as the current state of knowledge regarding methane hydrates R&D.

The review was prompted by UNEP's recognition of gas hydrates as an emerging global issue linked to both future energy supply and global environmental change. Natural gas hydrate systems are steadily gaining attention in the media and within the scientific, government, and industry communities, but many questions and issues associated with natural gas hydrates remain. As a result, the UNEP/Grid review of natural gas hydrate systems comes at the right time to present the current state of knowledge within these communities. This review highlights issues and areas that will require future attention in order to constrain and better understand the role of natural gas hydrates in the global climate cycle, their potential as a "lower-carbon" energy source, and related environmental and socio-economic issues.

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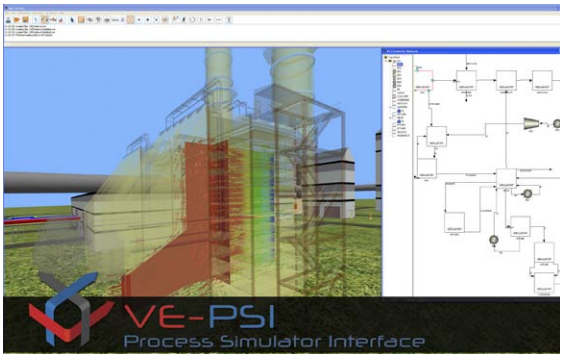



## Energy Plant Design Software Wins Award

The Federal Laboratory Consortium will award a 2010 Excellence in Technology Transfer Award to NETL for successfully making its innovative software technology, the Virtual Engineering -Process Simulator Interface (VE-PSI), available to the private sector and other government laboratories. The open-source software facilitates the collaborative design of next-generation energy plants within an immersive, interactive, three-dimensional, plant walk-through virtual environment. The capability enables quick, efficient, and inexpensive creation of virtual prototypes for new plant designs, thereby reducing the time and materials expended on pilot- and demonstration-scale plants. VE-PSI was developed by NETL in collaboration with Ames National Laboratory and Reaction Engineering International. The award will be presented to NETL researchers Stephen Zitney and Terry Jordan at the Consortium's annual national meeting on April 29 in Albuquerque, NM.

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

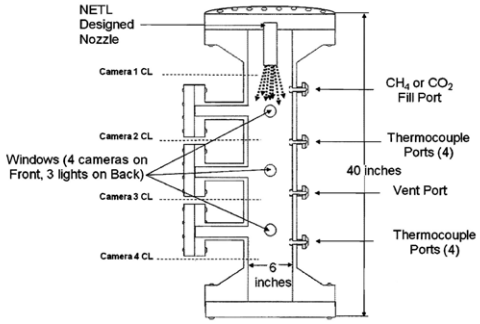
*Image depicting how EYESim™ works.*

## NETL Presents Advanced Energy Plant Operations, Future Training

NETL presented its vision of future plant operations and training for advanced energy systems at the 14th Annual ARC World Industry Forum. Plant operations can be improved through increased use of innovative computational tools, immersive virtual simulation, advanced real-time optimization and model predictive control solutions, wireless sensor networks, and enhanced self-diagnosis and decision-making tools.

This presentation emphasized real-time dynamic simulators with operator training system (OTS) capabilities, along with immersive training systems (ITS) that provide three-dimensional virtual plant walk-through environments for training field operators and engineers. It also highlighted NETL's Dynamic Simulator Research and Training (DSR&T) Center, which is scheduled to be launched in late 2010 with the deployment of a combined OTS/ITS solution for an IGCC reference plant with carbon capture. The plant-wide IGCC training system will make use of the Invensys Operations Management Dynsim™ software for the OTS and EYESim™ software for the ITS. EYESim™ was recently selected as a Breakthrough Product of 2009 by *Processing* magazine and was featured, along with NETL's DSR&T Center, in a recent *ARC Insights* article.

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

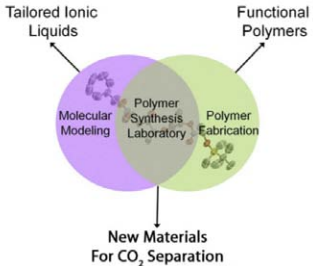



## New Technique to Form Methane Hydrate

Experiments at NETL have shown that rapid formation of methane (natural gas) hydrate, and other gas hydrates, is possible. The rapid hydrate formation process is made possible by use of a novel (U.S. Patent application in progress) nozzle which allows almost instantaneous and continuous formation of methane hydrate. The process occurs at temperatures between 5 - 15°C in a 900 psig methane environment. The process was conducted in the 15 L hydrate cell, also designed at NETL. Hydrate formation continued for several days while the flow rates and temperatures of the water and methane and the overall temperature of the methane environment were varied.

Raman Spectroscopy verified that Type I clathrate methane hydrate (the same type of methane hydrate that is found in nature) was formed using this process. Methane hydrate formation typically takes anywhere from a minimum of six hours to several days or weeks in the laboratory setting. Rapid and continuous methane hydrate formation allows a more cost-effective method for the storage and transport of methane compared with conventional compressed and liquefied natural gas. Methane hydrate has the ability to store 164 times its volume (at STP) in gas. The hydrates exhibit a self-preservation phenomenon that allows for the hydrate to be transported at atmospheric pressure and temperatures between -10 to -20 °C. This temperature range is the same as that used commercially to transport frozen foods in trucks, box cars, and ships, requiring no new transportation technology to be utilized for the hydrate transport. This has the potential to provide a tremendous cost savings over compressed and liquefied natural gas transportation.

Contact: Thomas D. Brown, 412-386-4691




## Polymer Synthesis Laboratory Focuses on Materials for $CO_2$ Capture and Conversion

A new facility is being used to develop synthetic methods and explore the physical and chemical attributes of functionalized materials and their interactions with $CO_2$ to make advanced materials for $CO_2$ capture and conversion. PSL scientists are collaborating closely with molecular modelers to develop $CO_2$ capture devices in an "atoms up" approach that creates materials tailored specifically for the application.

PSL work will be a fundamental component of the planned collaboration between NETL and the Berkeley Energy Frontier Research Center (EFRC), one of 46 DOE-supported EFRCs partially funded through the American Reinvestment and Recovery Act to address the full range of energy research challenges in renewable and carbon-neutral energy, energy efficiency, energy storage, and crosscutting science.

In one example of this type of collaboration, synthetic polymer chemists are working closely with membrane fabrication experts to improve support materials for ionic liquid membranes.

Contact: Dave Luebke, 412-386-4118

## Coal Seam Carbon Sequestration Simulation

The world's first enhanced coalbed methane/carbon sequestration field project took place in the Allison field in northwest New Mexico. A newly-developed model was used to investigate the roles of coal shrinkage and swelling, coal elastic properties, and cleat porosity and permeability, which together determine the geomechanical responses of the coal-seam system. The new model simulated coal permeability and gave a better fit to the field data than that obtained with earlier models. The results were used to estimate the "best" values for geophysical parameters that are difficult to measure in the laboratory. These findings were published in the journal of the Society of Exploration Geophysicists, *The Leading Edge*, vol. 29 (2010), pp. 224ff. The article is entitled, "Flow simulations for carbon sequestration at a coal-seam pilot site."

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

## Fluidized-Bed Combustion Testing

Detailed knowledge of bubble parameters is essential to understanding heat exchanger tubes erosion in fluidized-bed combustion units. Researchers from NETL, Argonne National Laboratory (ANL), and Foster Wheeler collaborated to investigate bubble parameters in fluidized-bed combustors. Foster Wheeler provided experimental differential pressure data obtained in a variable-thickness fluidized bed, and NETL and ANL used a two-phase computational fluid dynamics (CFD) hydrodynamic model to analyze and predict the data. The experimental results and predictions for autocorrelations, cross-correlations, power spectral densities, and bubble parameters, such as frequencies, velocities, and diameters, were in agreement.

This collaborative effort produced a paper that has been accepted for publication in *Industrial & Engineering Chemistry Research*. The manuscript, expected to be published in the June 2010 issue, is titled "Experimental and CFD Analyses of Bubble Parameters in a Variable-Thickness Fluidized Bed" and was authored by R. W. Lyczkowski, J. X. Bouillard, I. K. Gamwo, M. R. Torpey, and E. D. Montrone.

Contact: Isaac K. Gamwo, 412-386-6537

## Non-linear Fluid Models Aid in Oil Drilling

Non-linear fluid models can numerically calculate the velocity components, the pressure field, and shear stresses related to the drag force on an oscillating cylinder and are very important in oil-drilling applications. Recently, our researchers collaborated with the University of Kentucky to derive an explicit expression for the internal energy density and to demonstrate the existence of an entropy density function in these fluids. Thermodynamic restrictions on material functions and stress coefficients that appear in generalized second grade fluid models were obtained. The results were recently published by C. S. Man and M. Massoudiin *Continuum Mechanics and Thermodynamics*, vol. 22 (2010), pp. 27-46.

Contact: Mehrdad Massoudi, 412-386-4975

## Hydraulic Compression Technology Evaluated for $CO_2$ Sequestration Applications

Simulation studies are being conducted on the possible advantages of using hydraulic compression to compress $CO_2$ prior to geologic sequestration. In hydraulic compression, a circulating column of water is used to compress bubbles of gas introduced near the top of the column. The entrained bubbles are compressed as the gas/water mixture descends, and then separated from the water in a large chamber at the bottom of the column. At this point, the compressed gas is collected and the circulating water is returned to the top of the column.

Anticipated compression efficiencies would approach that of isothermal compression. The potential energy savings are about one-third relative to conventional intercooled turbo-compressors and have a corresponding cost reduction.

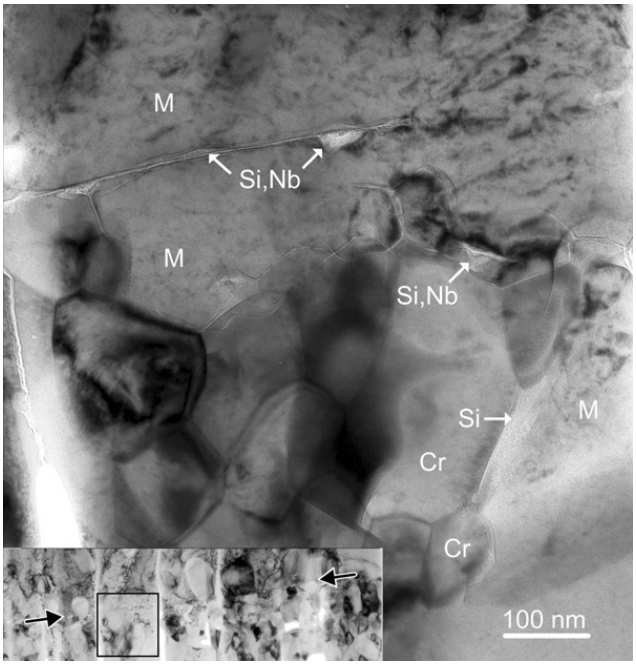
Contact: Edward L. Parsons, 304-285-4533

## New Model Developed for SOFC Electrode

A model describing the transport of charge through a solid oxide fuel cell (SOFC) electrode via two pathways (surface oxygen-ion transport and bulk electrode oxygen vacancy transport) was developed by researchers at NETL and West Virginia University. The model assumes separate voltage losses as charge transfers occur at the 2-phase boundary (2PB) between the cathode and electrolyte, and at the 3-phase boundary (3PB) between the cathode, electrolyte, and gas phase.

Using diffusion transport models for the surface oxygen-ions and bulk vacancies, the model provides information on the relative transport of charge. Results show that in fuel cell mode, when voltage differences are low, 3PB current dominates. The 2PB current becomes more important with increasing differences in voltage. In electrolysis mode, 2PB current is very small compared with 3PB. This result aligns with recent work presented in the literature and suggests that to study 3PB current, the cell needs to be operated in electrolysis mode. This work was presented at the recent American Ceramic Society meeting in Daytona Beach, FL.

Contact: Randall Gemmen, 304-285-4536




*A low magnification BF TEM image of the foil is shown in the inset. The scale/metal interface appears linear (indicated by the arrows). Note that the broad, nearly vertical linears are due to thinning. A higher magnification image of the indicated area (box) revealed an amorphous Si-rich layer at the scale/metal interface. This layer also encapsulated several chromia grains within the first 250 nm of the scale. The width of the Si-rich layer in both regions is approximately 10 nm. The various indicated areas are M=metal matrix, Cr=chrome rich oxide, Si=silicon rich oxide, and Si,Nb=silicon rich oxide with some Nb.*

## Metallic Interconnects Perform

NETL researchers are investigating the use of ferritic stainless steel alloy 441 as an inexpensive metallic interconnect. Interconnects are ceramic or metallic layers that connect the various components of a solid oxide fuel cell. These interconnects have to be resistant to both oxidizing and reducing conditions and highly conductive to electricity. Alloy 441 was chosen because it is both commercially available and relatively inexpensive. Most commercial ferritic stainless steels form a resistive silica-rich subscale. Researchers originally thought that this alloy did not form silica scale. However, recent research has now shown that, in fact, the alloy does form a silica-rich subscale, but the subscale is conductive. These results were recently published in the *Journal of Power Sources*, vol. 195 pp. 813-820.

Contact: Paul D. Jablonski, 541-967-5982

## EPA Chooses NETL Model for National Standard

To determine the level of reduction in greenhouse gases (GHG) that can be expected from compliance with Renewable Fuel Standards, EPA is referring to the NETL life-cycle analysis of petroleum-based transportation fuels. Selected for its accuracy and transparency, the NETL study provides a comprehensive baseline of GHG emissions generated over the life cycle of conventional petroleum-based transportation fuels (i.e., gasoline, diesel fuel, and kerosene-based jet fuel) in the United States. The study also identifies GHG reduction opportunities in each life-cycle stage of the conventional fuels.

According to the EPA final rule on the recently revised Renewable Fuel Standard Program, the volume of renewable fuels that refiners and importers are required to phase into their products will be based on GHG reduction goals measured from the NETL 2005 life cycle baseline. The NETL petroleum baseline report and underlying Microsoft Excel model are both publicly available at the NETL website. Collaboration with the EPA Office of Transportation and Air Quality over the past two years has established NETL as a leader in the field of life-cycle analysis while strengthening the DOE-EPA working relationship.

Program Contact: Timothy Skone, 412-386-4495

## Appliance Technology Tested for Standby Power Consumption

The Appliance Technology Evaluation Center at NETL recently completed a series of non-active power consumption (OFF and standby modes) tests on 14 dishwashers, 13 dehumidifiers, and 32 cooking appliances (ranges, ovens, cook tops). The operating control on each of the 58 appliances was evaluated for technology content and cost. The standby power and control evaluation data will be used by DOE's Rulemaking Team for Appliance Technology to create the first standby power consumption standard for these products. The standby test will be added to the applicable appliance test procedures.

Contact: Donald Ferguson, 304-285-4192

## NETL Assesses Thermodynamics of Selected Refractory Alloys

Refractory metal-based alloys are of great importance due to their usefulness in ultra-high temperature fossil energy plant applications. Chromium is of particular interest due to good oxidation resistance, low density (20% less than most nickel-based superalloys) and high thermal conductivity (two to four times higher than most superalloys). However, low ductility and fracture toughness of chromium and its alloys at room temperature prevent them from becoming a viable material for advanced fossil energy applications. The addition of the rare earth elements in small amounts can increase both ductility and creep resistance of refractory metal-based alloys.

NETL researchers investigated the binary phase diagrams of chromium with the rare-earth elements yttrium, cerium, and lanthanum to obtain thermodynamic quantifications that could be used in process control, microstructure optimization, and kinetics simulations.

The results of this study appear in the *Journal of Phase Equilibria and Diffusion*, (Vol. 30, No. 6, pp 578ff.).

Contact: Ömer Doğan, 541-967-5858

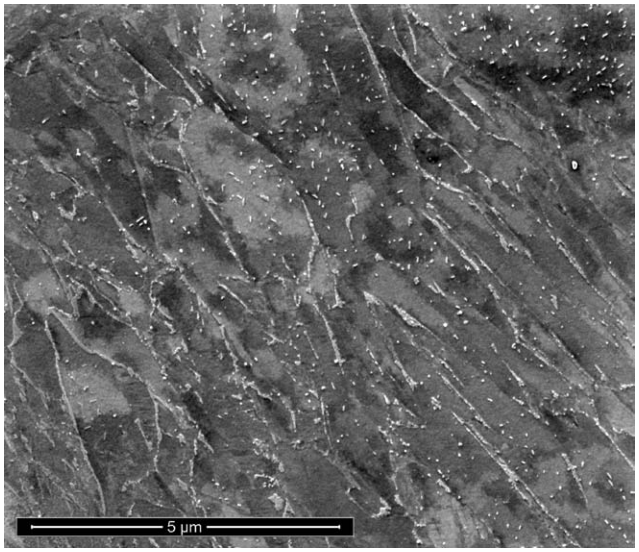
## Tracers Track the Subsurface Movement of $CO_2$ at Test Site

Perfluorocarbon tracers successfully detected underground migration of $CO_2$ at the San Juan Basin pilot sequestration test site in northern New Mexico. Two different perfluorocarbon tracers were added sequentially to $CO_2$ during the first two months of injection in September and October 2008. The tracers, which can be measured at concentrations of parts-per-quadrillion, were detected in the production gas at the east offset well, peaking in February 2009, and at the southwest offset well in June 2009. The tracer measurements provided the first evidence of subsurface migration of the plume; simultaneous monitoring of $CO_2$ at the same locations was not sensitive enough to detect the change.

Numerical models based on limited subsurface characteristics data had predicted the migration; however, breakthrough at the southwest well was expected to be first, in contrast to the field measurements. The tracer results are being used to refine the models and to better understand the subsurface $CO_2$ migration pathways.

The perfluorocarbon monitors were located at three offset production wells about 400 meters from the injection well.

Contact: Arthur W. Wells, 412-386-5975




*A Secondary Electron image showing the as-cast martensitic microstructure of one of the newly-developed, high-temperature Fe-based alloys.*

## Thermodynamic Modeling Used to Select Iron Alloys for Testing

NETL researchers are attempting to eliminate sources of microstructural instability typically found in the ferritic/martensitic alloys currently used in most coal-fired power plants. Based on ThermoCalc modeling of 19 iron-based alloy compositions, the researchers were able to select three new and unique compositions that have the potential to outperform currently available alloys. The new ferritic/martensitic Fe-based alloys are targeted to withstand temperatures to 650°C, which will enable them to be used in higher efficiency power plants. Tremendous cost savings are possible since the austenitic iron and nickel-based alloys and superalloys currently used in such applications are much more expensive. The three alloy compositions have been formulated from high purity meltstock and will be melted, cast, and fabricated for future testing.

Contact: Chris Cowen, 541-967-5952)

## NETL Method Measures Subsurface Water Interaction with Coal Utilization By-product (CUB)

Using strontium (Sr) isotopes, NETL scientists quantified the extent to which mine water interacts with CUB-containing grout used in remediation at the inactive Omega Coal Mine in West Virginia. The grout consisted of 98 percent fluidized-bed combustion ash and fly ash with 2 percent Portland cement. The ratio of strontium isotopes (87Sr/86Sr) in the mine water clearly distinguished discharges from grouted and non-grouted areas, whereas conventional chemical analysis could not. Based on results of the study, water that interacted with the grout received 30–40 percent of its strontium from the grout mixture, suggesting the grout is chemically eroding at a rate of approximately 0.04 percent per year. The same approach is now being used to study the interaction of sub-surface $CO_2$-laden waters with geologic media at carbon sequestration sites. The February issue of the Elsevier journal *Applied Geochemistry* (Vol. 25 (2010), No. 2, pg. 212ff.) describes the study.

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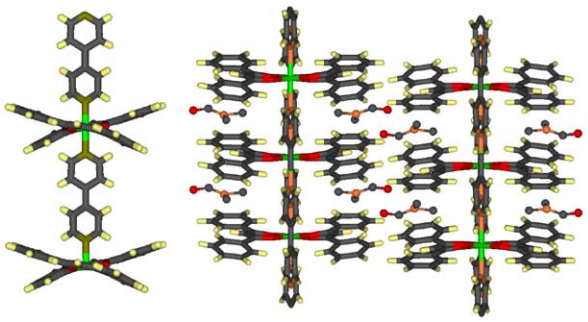
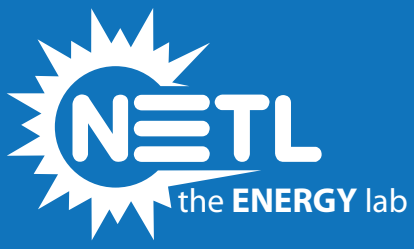


*The as reported by Soldatov et al.54 Left, a view showing an isolated chain of Ni-DBM-BPY. Right, a view showing the packing arrangement of the chains with DMF guests located in the interchain voids. Key: C, gray; H, yellow; O, red; N, orange; Ni, green.*

## NETL Researchers Investigate Sorbent for the Selective Adsorption and Capture of $CO_2$

Researchers at NETL have identified how small molecules such as $CO_2$ and $CH_4$ are adsorbed in a porous sorbent that undergoes selective structural changes when exposed to different gases. The gas-induced structural transformations give these solid sorbents the potential to adsorb a specific gas from a mixed stream based on process temperature and pressure. This capability could be used to capture $CO_2$ from mixed flue gas streams or to improve the BTU content of natural gas by removing $N_2$, $CO_2$, and other impurities. The technique used to study adsorption-desorption cycles at pressures up to 30 atmospheres with a modified infrared spectrometer has given the researchers new insight into the performance of these novel sorbents, and it is described in the *Journal of Physical Chemistry C* (Vol. 114 (2010), No. 2, pg. 2184ff.) published by the American Chemical Society.

Contact: Christopher Matranga, 412-386-4114

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