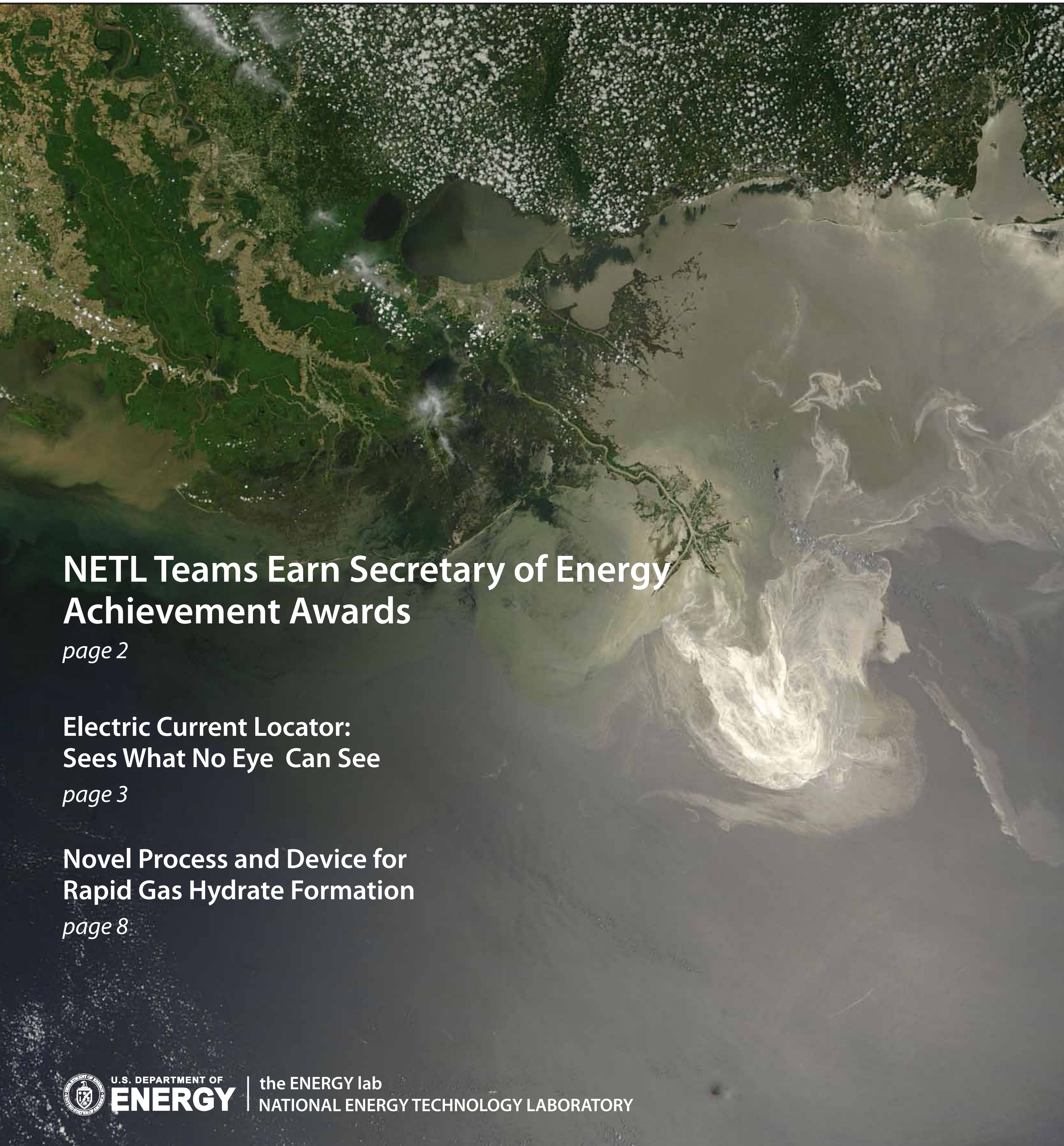
netlognews

NETL's R&D newsletter

January 2012, Issue 24



NETL Teams Earn Secretary of Energy Achievement Awards

page 2

Electric Current Locator: Sees What No Eye Can See

page 3

Novel Process and Device for Rapid Gas Hydrate Formation

page 8

U.S. DEPARTMENT OF ENERGY | the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

Contents

Cover image: The Deepwater Horizon spill as seen by NASA's Terra satellite on May 24, 2010.

netlognews

newlognews is a quarterly newsletter that 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.

Award recipients for DOE's remediation activities at the Hanford nuclear production site.

Award recipients for Deepwater Horizon oil spill in the Gulf of Mexico efforts.

NETL Teams Earn Secretary of Energy Achievement Awards—On October 27, Secretary of Energy Stephen Chu honored the National Energy Technology Laboratory (NETL) and several partner agencies with two Secretary of Energy Achievement Awards, the highest nonmonetary awards an employee or contractor can receive from DOE. NETL and its partners will be recognized for contributions to two significant environmental efforts in 2010: the Deepwater Horizon oil spill in the Gulf of Mexico and DOE's remediation activities at the Hanford nuclear production site.

NETL was recognized for its swift and effective response to the Deepwater Horizon oil spill, perhaps the worst environmental disaster to have occurred in the United States. The Incident Command's Flow Rate Technical Group/ Nodal Analysis Team was led by NETL's Dr. George Guthrie and staffed by researchers from NETL, Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Pacific Northwest National Laboratory, Oak Ridge National Laboratory, and the National Institute of Standards and Technology. This multiagency effort was critical to estimating the rate of oil flowing into the Gulf and, in turn, to developing options to cap the well. Their analysis guided key decisions, helping to speed the ultimate solution and reduce the environmental cost of the disaster.

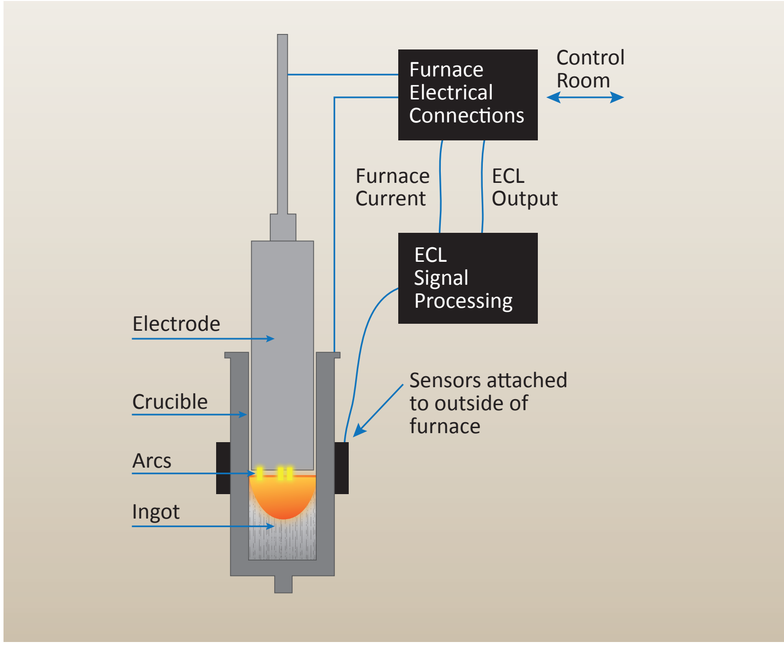
At the Hanford Site in the state of Washington, nine nuclear reactors and their associated facilities produced plutonium for our nation's defense during World War II and throughout the Cold War. Today, the site is home to one of the most complex and challenging environmental clean-up projects in our nation's history.

An NETL team of recognized experts in computational fluid dynamics evaluated Bechtel National Inc.'s (BNI's) pulse-jet mixing vessel design to ensure that the system is safe, secure, and sound. The vessel was developed for the waste treatment and immobilization plant that BNI is designing and building at the site. The plant will be the world's first chemical processing facility capable of turning radioactive liquid waste into a stable glass form suitable for safe, permanent disposal. The pulse-jet mixing system is designed to safely process the 53 million gallons of liquid nuclear waste stored in aging tanks at the site today.

Electric Current Locator: Sees What No Eye Can See

—Vacuum arc remelting (VAR) is a crucial step in creating metals and alloys with the advanced properties needed for the aerospace, power generation, defense, medical, and nuclear industries. The problem is that the metal ingots produced occasionally contain defects, but who can see within the enclosed crucible of the furnace to know what causes these defects?

The new electric current locator (ECL) can "see" where eyes cannot. Developed under an agreement between NETL and the Specialty Metals Processing Consortium, the ECL tracks the positions of the electric arcs inside the VAR furnace in real-time. Knowing where the arcs are shows how energy is being distributed to the molten metal during the remelting process. "Seeing" the arcs is a first step toward controlling them and thereby controlling the melting process, which is necessary for consistently defect-free materials.



Sensors for the ECL, placed outside the furnace, can "see" through walls

Initially envisioned as a monitoring device for processes such as VAR, the ECL technology can easily be retrofitted to existing furnaces. The technology has been successfully applied to an industrial VAR during commercial production of a titanium alloy, during which some previously unreported aspects of arc behavior were identified and described in publications. For instance, the VAR showed that different patterns of arc distribution can arise for different melts, even though the same alloy is being melted using the same control program. These differences were not detectable by previous furnace controls. A patent application for the ECL has been filed, and NETL is looking for commercial partners to refine the technology and license it for commercial applications.

Contact: Charles (Rigel) Woodside, 541-967-5879

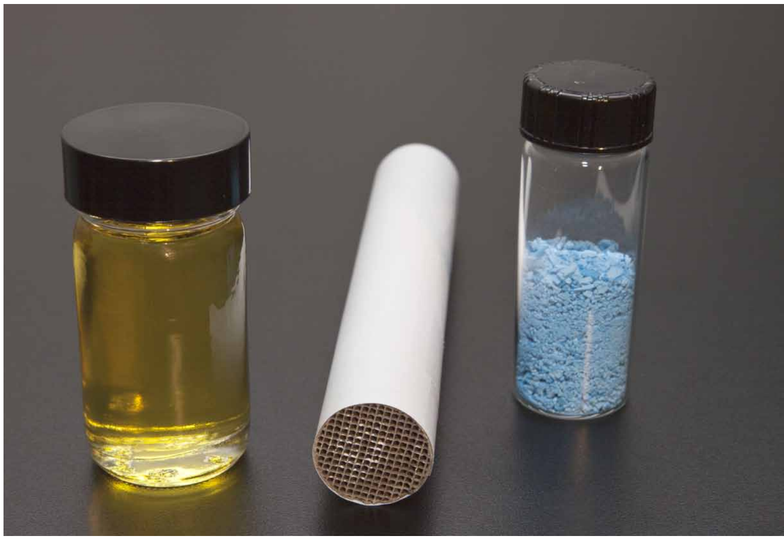
Dr. Jairo Valdes-Ortiz (left) discusses progress with Dr. Paul Jablonski on identification of macro-defects in nickel alloys melted by the vacuum arc remelting process.

Former NETL ORISE Student Wins Award—Dr. Jairo Valdes Ortiz, a Fulbright Scholar and ORISE (Oak Ridge Institute for Science & Education) student at NETL in 2010, won the best student paper award at the Materials Science and Technology (MS&T) 2011 Conference and Exhibition, held October 16-20, 2011, in Columbus, Ohio. The paper, titled "On the Formulation of a Freckling Criterion for Ni-Based Superalloy Vacuum Arc Remelting Ingots," discussed his work at NETL on predicting the presence of "freckling" or defects observed in large superalloy ingots used to create gas turbine parts. The results of this research could lower the chance of defects when casting the ingots, thus decreasing the number of ingots rejected during the process.

During vacuum arc remelting (VAR), metal ingots produced occasionally contain defects, which render them unusable. In experiments using a tilted surface on which the nickel-based alloy could solidify within the VAR, Dr. Ortiz determined that the tilted surface helps change the orientation of channels that generally lead to freckling. By controlling how energy passes through the alloy during the melting process, he made an important step toward defect-free materials.

The MS&T partnership of four leading materials societies—ACerS, AIST, ASM, and TMS—brings together scientists, engineers, students, policy makers, suppliers, and more to discuss current research and technical applications and to shape the future of materials science and technology.

Dr. Ortiz participated in the ORISE program while pursuing his Ph.D. in materials science at West Virginia University.



Incorporating active metals into the crystal structure of pyrochlore minimizes catalyst poisoning.

Novel Catalyst Technology Helps Convert Diesel to Syngas—Methods for generating synthesis gas from simple hydrocarbons such as methane routinely involve the use of a catalyst. However, the high sulfur and aromatic content of fuels such as diesel poses a major challenge, since these components can deactivate conventional catalysts. Unfortunately, no economically feasible reforming catalyst is available for converting diesel and coal-based fuels into hydrogen-rich synthesis gas necessary for use in solid oxide fuel cells.

To minimize catalyst poisoning while maintaining high activity, NETL researchers developed the novel idea of incorporating active metals into the crystal structure of a thermally stable material: pyrochlore. The unique crystalline structure of pyrochlore allows for chemical modifications tailored to specific fuels and reaction conditions. Development of this technology has resulted in two patent-pending inventions, one for utilization of pyrochlore catalysts in hydrocarbon reforming processes and the other for a method of optimizing the performance of pyrochlore catalysts for a particular application or specific operating condition. Together, these inventions help overcome the limitations of current catalysts by efficiently reforming diesel fuel while maintaining thermal stability and resistance to sulfur, aromatics, and carbon formation.

The commercial potential of these inventions has recently been recognized through the execution of an exclusive licensing agreement with the newly-formed Pyrochem Catalyst Corporation. This agreement marks the first time that an NETL-licensed technology has been used as a basis for the creation of a start-up company. The successful commercialization of pyrochlore-type catalysts for reforming hydrocarbon fuels may lead to the creation of high-technology jobs.

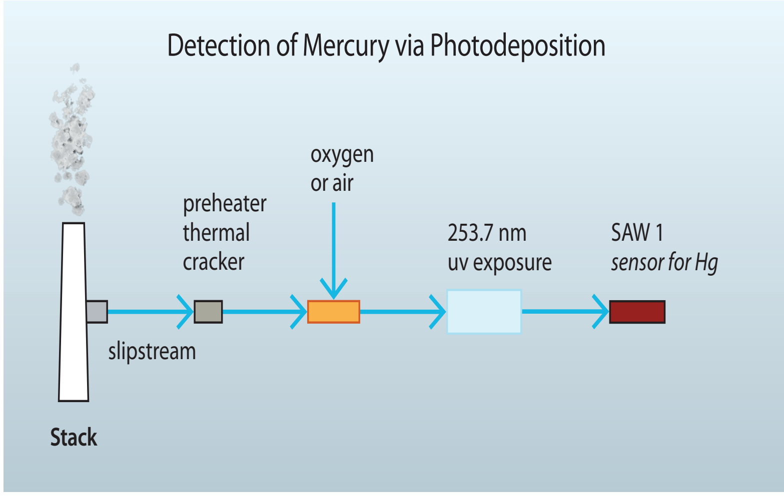
Contact: David Berry, 304-285-4430

NETL Develops Technique for Detection of Mercury

—The U.S. Environmental Protection Agency issued a national regulation for mercury removal from coal-derived flue and fuel gases on December 21. In addition, many states are promulgating their own rules for mercury emissions from coal-burning power plants. These rules typically require 90 percent or greater levels of capture of mercury. The levels of mercury in untreated coal-derived flue gas are on the order of 1 part-per-billion (ppb) by volume. Ninety percent removal requires treated flue gas with levels of 0.1 ppb, which in a dirty complex matrix can be difficult to measure, especially on a near continuous basis.

Methods for detection of mercury in coal-derived gas streams are needed to insure compliance with emission regulations. The potential market for mercury analyzers in application to coal-utilizing facilities in the United States is estimated to be in excess of $100 million.

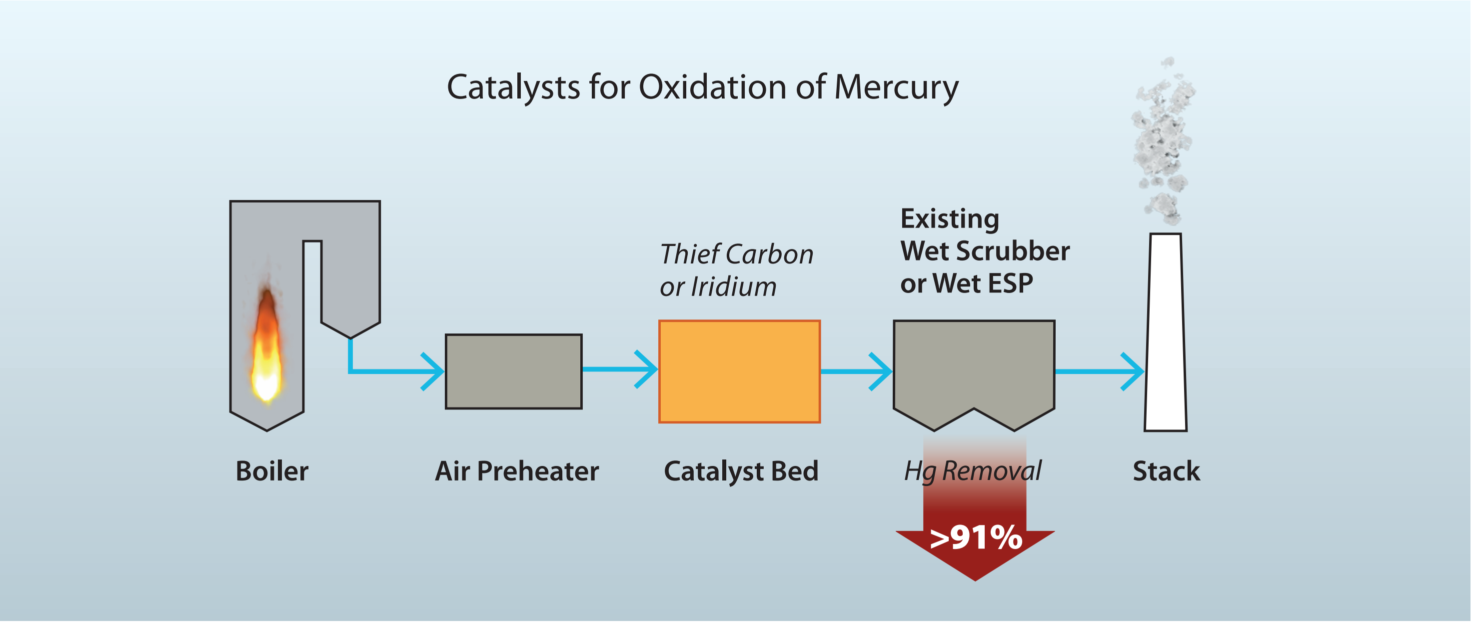
The NETL-developed and patented GP-254 process, introduces ultraviolet light at a wavelength of 254 nanometers into the flue gas, resulting in the conversion of elemental mercury to a more readily captured oxidized form. Oxidized forms of mercury tend to condense or photo-deposit on fly ash and activated carbon particles.



Schematic depiction of the invented detection process in accordance with features of the present invention. An array of Surface Acoustic Wave (SAW) sensors can be used where each sensor semi continuously monitors emissions of a particular heavy metal or metalloid.

This can facilitate the removal of mercury upstream of a particulate collection device such as an ESP or baghouse, as well as capture in a wet scrubber. Photo-deposition can also serve as the basis for pre-concentration and detection of small quantities of mercury within various gas streams, through mass, colorimetric, conductivity, UV absorption or UV fluorescence sensors. The technology, "Semi-continuous detection of mercury in gases," is described in U.S. Patent 8,069,703 issued in December 2011 and is a spin-off from the GP-254 Process. These findings are summarized in recent papers in the journals *Industrial & Engineering Chemistry Research, Fuel Processing Technology,* and *Energy & Fuels.*

Contacts: Evan J. Granite, 412-386-4607 and
Henry W. Pennline, 412-386-6013



Mercury is oxidized in a catalyst bed by Thief carbon or iridium. Mercury oxide removal is then facilitated in existing wet scrubber or wet ESP.

Catalysts Developed for Oxidation of Mercury in Coal-Burning Power Plants—The U.S. Environmental Protection Agency issued a national regulation for mercury removal from coal-derived flue and fuel gases in excess of 90 percent on December 21. Levels of mercury in untreated coal-derived flue gas are on the order of 1 part-per-billion (ppb) by volume; 90 percent removal requires treated flue gas with levels of 0.1 ppb, which can be difficult to obtain. The predominant species of mercury in low-rank coal-derived flue gases is the elemental form, Hg(0), which, because of its relative inertness and insolubility in water, is challenging to remove and not captured efficiently by many activated carbons.

Mercuric chloride is highly soluble in water and is more readily removed by carbon. A catalyst that can oxidize elemental mercury to mercuric chloride (or another compound) would be of tremendous value. A catalyst would enable mercury to be captured by existing air pollution control devices (APCDs) present in coal-burning power plants. These existing APCDs include wet scrubbers for acid gas removal, as well as electrostatic precipitators (ESPs) and bag house filters for particulate removal.

Several materials have been previously proposed as catalysts for oxidation of mercury including palladium, gold, platinum, SCR catalysts, fly ash, activated carbons, and halogen compounds. NETL researchers recently discovered that iridium and "Thief" carbons are excellent catalysts for the oxidation of mercury in flue gas. These findings are summarized in recent papers in the journals *Environmental Science & Technology, Energy & Fuels, and Platinum Metals Review*,and in several U.S. patents.

The "Thief" carbons are active for the oxidation of mercury and, if desired, are cheap enough to be a disposable catalyst. The catalyst technology is available for license and is a spin-off from the 2009 R&D 100 Award-winning Thief Process developed at NETL.

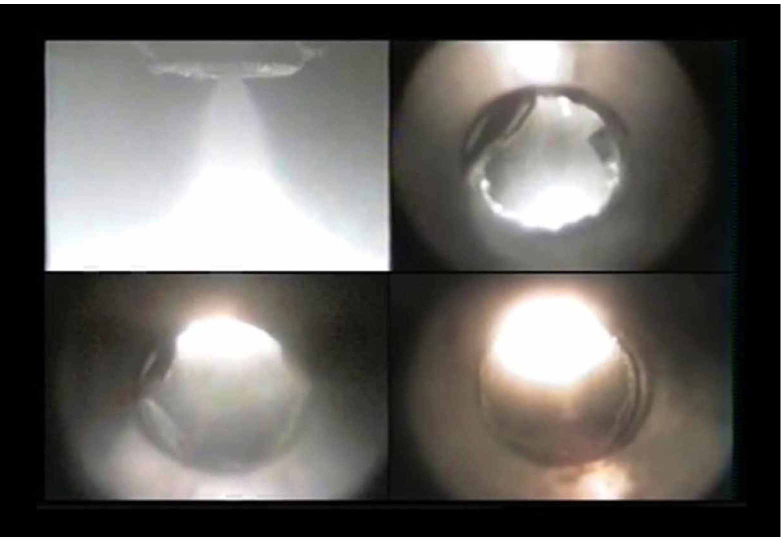
Contacts: Evan Granite, 412- 386-4607, and
Henry Pennline, 412-386-6013

Parr autoclave system used in corrosion measurement.

New Method Identified For Measuring Corrosion Rates of Metals and Alloys in Low Electric Conductivity Environments—Corrosion behavior of alloys in low-conductivity environments using reliable, time-efficient in-situ electrochemical methods has recently been studied by researchers from the Pennsylvania State University and NETL. They have determined the corrosion rates of carbon steels in supercritical CO_2 undersaturated with water, a low electric conductivity environment, using three independent electrochemical methods (linear polarization, electrochemical impedance spectroscopy, and electrochemical frequency modulation). The conditions of the corrosion tests were at 50 °C and 10 MPa with a water concentration of 2000 ppm, half the water saturation limit for supercritical CO_2. The results were repeated in duplicative tests that generated reproducible results.

This type of electrochemical measurement has never before been performed in this environment. It was accomplished in part by the innovative use of a highly conductive film as the electrolyte that allowed for measurements to be carried out in the otherwise very low electric conductivity environment. With further development, the results could be used not only to predict alloy performance in these environments but could lead to a new class of corrosion sensors for monitoring alloys' corrosion performance in low electric conductivity environments encountered in fossil-fueled power plants and in CO_2 transport and storage facilities.

Contacts: Margaret Ziomek-Moroz, 541-967-5943, and
Gordon Holcomb 541-967-5874



The tip of the nozzle is located just above the top viewing window in the top left quadrant of this video still. This series of images shows hydrate formation in the 15 Liter view cell through the view cell's 4 portholes. Upper left, hydrate formation at the nozzle, upper right, lower left, and lower right are hydrate "snow" at the 2nd, 3rd, and 4th porthole.

NETL's rapid hydrate formation process allows instantaneous and continuous methane hydrate formation by use of a novel nozzle. The nozzle is located at the top where the flange begins to taper in.

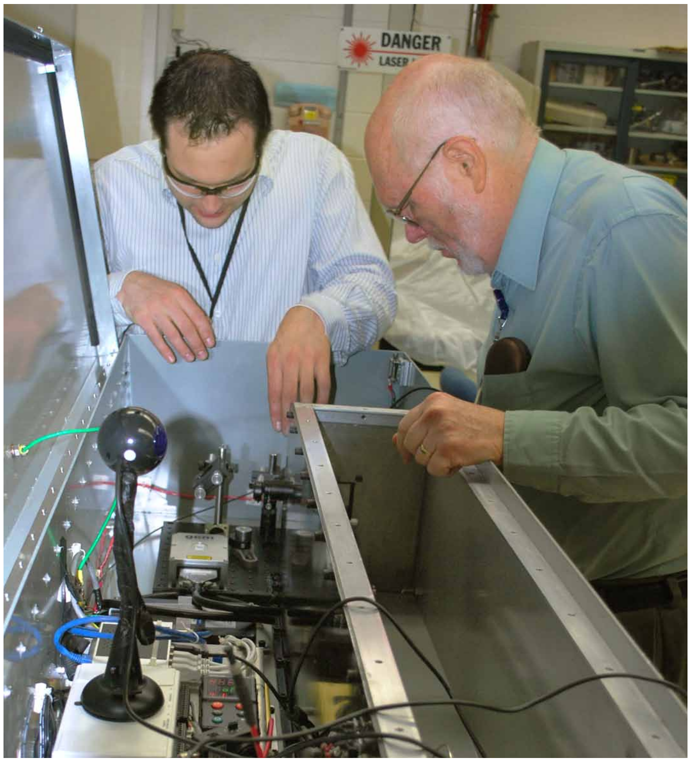
Novel Process and Device for Rapid Gas Hydrate Formation—The results of recent research at NETL show that rapid and continuous formation of methane (natural gas) hydrate, as well as other gas-derived hydrates, is achievable. This technology will provide a safer and potentially lower-cost alternative for natural gas storage and transportation.

Methane hydrate formation typically takes anywhere from six hours to several days or weeks under laboratory conditions. However, NETL's rapid hydrate formation process allows instantaneous and continuous methane hydrate formation using a novel nozzle. This patent-pending technology produces gas hydrates from a mixture of water and a hydrate-forming gas. The two-phase mixture is created within the spray nozzle. The mixture is subsequently sprayed into a reaction vessel, under pressure and temperature conditions suitable for gas hydrate formation. Because the reaction zone pressure is less than the mixing zone pressure, the expansion of the hydrate-forming gas in the mixture provides a degree of cooling and optimal mixing, while allowing for improved gas solubility and heat transfer.

Gas hydrates have the potential to provide a tremendous cost savings over the transport of compressed and liquefied natural gas. In addition, this technology may be applicable to carbon dioxide sequestration, separation of mixed gases (e.g., natural gas streams containing carbon dioxide and other gases impacting higher methane content), cold energy storage, transportation fuels, and desalination processes. Also, reduced capital and operational costs for small to mid-sized gas fields make the adoption of gas hydrate more attractive to commercial interests.

NETL is currently seeking collaborative research and licensing partners for this technology.

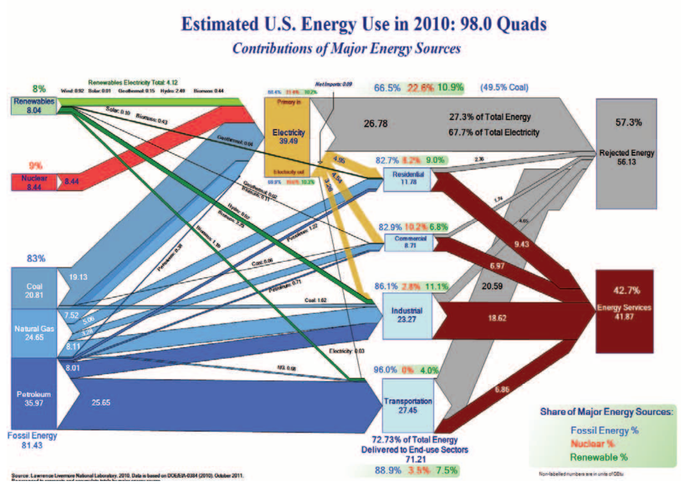
Contacts: Charles Taylor, and Thomas Brown



NETL researcher Dr. Michael Buric & Dr. Steven Woodruff assembling the gas composition sensor.

Raman Gas Composition Sensor Undergoes Field Test—A unique gas composition sensor emerging from collaboration between NETL and the University of Pittsburgh, a participant in the NETL-Regional University Alliance, is being evaluated for commercial gas turbine operation at the GE Gas Turbine Test Laboratory facility in Greenville, SC. Development of the sensor is a principal activity under a Cooperative Research and Development Agreement between GE and NETL. The sensor features a metal-lined capillary sampling tube that acts like a mirrored waveguide to greatly enhance weak Raman light scattering signals, allowing near-instantaneous analysis of gaseous mixtures with high-accuracy. Real-time gas composition analysis will allow feed forward data to control systems for power equipment such as gas turbines and fuel cells to achieve optimal performance with such fuels as coal-derived syngas, coal-bed methane, biogas, and natural gas.

Contact: Steven Woodruff, 304-285-4175



Click here for larger image

New Diagrams Illustrate How Energy Flowed in 2010—NETL energy analysts have produced for the public a set of Sankey diagrams based on data obtained from the Annual Energy Review 2010 recently released by the U.S. Energy Information Administration. Graphically representing both quantity and direction, the diagrams place in perspective the relative contributions of major domestic energy sources as well as the flow of fossil fuels around the world.

The "Estimated U.S. Energy Use in 2010" flow diagram shows the quantity of fuels used to drive each of the sectors in the United States. Overall, 83 percent of the primary energy consumed in the U.S. is from fossil fuels and downstream, due to conversion efficiencies, 89 percent of the total energy delivered to the end-used sectors is derived from fossil fuels.

The global Energy Related Flow Diagrams show major international flows of various fuels and identify who the major exporters/importers are in the global fuel market.

Contact: Erik Shuster, 412-386-4104

Recent NETL Publications

1.	Kutchko, B.G., Strazisar, B.R., Hawthorne, S.B. et al. July 2011. H(2)S-CO_2 Reaction With Hydrated Class H Well Cement: Acid-Gas Injection and CO_2 Co-Sequestration, *International Journal of Greenhouse Gas Control*, 5 (4) 880-888.
2.	Kobos, P.H., Cappelle, M.A., Krumhansl, J.L., et al. July 2011. Combining Power Plant Water Needs and Carbon Dioxide Storage Using Saline Formations: Implications For Carbon Dioxide and Water Management Policies, *International Journal of Greenhouse Gas Control*, 5 (4) 899-910.
3.	Goodman Angela; Hakala Alexandra; Bromhal Grant; et al. July 2011. US DOE Methodology For the Development of Geologic Storage Potential For Carbon Dioxide at the National and Regional Scale, *International Journal of Greenhouse Gas Control*, 5 (4) 952-965.
4.	Eslick, J.C., Miller, D.C. August 10, 2011. A Multi-Objective Analysis For the Retrofit of a Pulverized Coal Power Plant with a CO_2 Capture and Compression Process, *Computers & Chemical Engineering*, 35 (8) Special Issue: SI, 1488-1500.
5.	Zhang, Y., Vouzis, P., Sahinidis N.V. August 10 2011. GPU Simulations For Risk Assessment in CO(2) Geologic Sequestration, *Computers & Chemical Engineering*, 35 (8) Special Issue: SI 1631-1644.
6.	Choi, J-H, Seol, Y., Boswell, R., et al. September 8 2011. X-ray Computed-Tomography Imaging of Gas Migration in Water-Saturated Sediments: From Capillary Invasion to Conduit Opening, *Geophysical Research Letters*, 38 Article Number: L17310.
7.	Najera, M., Solunke, R., Gardner, T., et al. September 2011. Carbon Capture and Utilization Via Chemical Looping Dry Reforming, *Chemical Engineering Research & Design*, 89 (9A) Special Issue: SI, 1533-1543
8.	Holloway William; Benyahia Sofiane; Hrenya Christine M.; et al. October 1, 2011. Meso-Scale Structures of Bidisperse Mixtures of Particles Fluidized by a Gas, *Chemical Engineering Science*, 66 (19), Special Issue: SI, 4403-4420
9.	Syamlal, M., October 1, 2011. A Hyperbolic Model for Fluid-Solids Two-Phase Flow, October 1, 2011. *Chemical Engineering Science*, 66 (19) Special Issue: SI, 4421-4425.
10.	Monazam, E.R., Shadle, L.J., Siriwardane, R. October 5, 2011. Performance and Kinetics of a Solid Amine Sorbent for Carbon Dioxide Removal, *Industrial & Engineering Chemistry Research*, 50 (19), 10989-10995.
11.	Miller, D.D., Siriwardane, R., Simonyi, T. October 2011. Theoretical and Experimental Analysis of Oxygen Separation from Air over Ni-Transition Metal Complexes, *Energy & Fuels*, 25 (10), 4261-4270.
12.	Yang, Y-M, Small,M.J., Junker, B., et al. October 2011. Bayesian Hierarchical Models for Soil CO_2 Flux and Leak Detection at Geologic Sequestration Sites, *Environmental Earth Sciences*, 64 (3), 787-798.
13.	Poulston, S., Granite, E.J., Pennline, H.W.; et al. October 2011. Palladium Based Sorbents for High Temperature Arsine Removal From Fuel Gas, *Fuel*, 90 (10), 3118-3121.

Recent NETL Publications

14.	Li, T., Grace, J., Shadle, L., et al. November 15, 2011. On the Superficial Gas Velocity in Deep Gas-Solids Fluidized Beds, *Chemical Engineering Science*, 66 (22), 5735-5738.
15.	Dillon, S.J.; Helmick, L., Miller, H.M., et al. November 2011. The Orientation Distributions of Lines, Surfaces, and Interfaces around Three-Phase Boundaries in Solid Oxide Fuel Cell Cathodes, *Journal of the America Ceramic Society*, 94 (11) 4045-4051.
16.	Monazam, E.R., Shadle, L.J., Siriwardane, R., November 2011. Equilibrium and Absorption Kinetics of Carbon Dioxide by Solid Supported Amine Sorbent, *AICHE Journal*, 57 (11) 3153-3159.
17.	Li, T., Dietiker, J-F.; Zhang, Y., et al. December 1, 2011. Cartesian Grid Simulations of Bubbling Fluidized Beds With a Horizontal Tube Bundle, *Chemical Engineering Science*, 66 (23), 6220-6231.
18.	Karthik, S. Diwekar, U., Zitney, S.E. December 14, 2011. Stochastic Modeling and Multi-Objective Optimization for the APECS System, *Computers & Chemical Engineering*, 35 (12), 2667-2679.
19.	Yue, W., Babatunde, B., Kun, L., et al. December 15, 2011. Experimental Measurements and Equation of State Modeling of Liquid Densities for Long-Chain N-Alkanes at Pressures to 265 MPa and Temperatures to 523 K, *Fluid Phase Equilibria*, 311, 17-24.
20.	Tsai, A., Tucker, D., Clippinger, D. December 2011. Simultaneous Turbine Speed Regulation and Fuel Cell Airflow Tracking of a SOFC/GT Hybrid Plant With the Use of Airflow Bypass Valves, *Journal of Fuel Cell Science and Technology*, 8 (6) Number: 061018.

Patents Issued

1.	Semi-Continuous Detection of Mercury in Gases, Evan J. Granite and Henry W. Pennline, Patent number 8,069,703, issued December 6, 2011.
2.	Thief Carbon Catalyst for Oxidation of Mercury in Effluent Stream, Evan J. Granite and Henry W. Pennline, Patent number 8,071,500, issued December 6, 2011.
3.	Method for the Production of Mineral Wool and Iron from Serpentine Ore, William K. O'Connor, Gilbert Rush, and Glen F. Soltau, Patent number 8033140, issued October 11, 2011.

National Energy Technology Laboratory
1450 Queen Avenue SW
Albany, OR 97321-2198
541-967-5892

2175 University Avenue South
Suite 201
Fairbanks, AK 99709
907-452-2559

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4764

626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4687

Granite Tower, Suite 225
13131 Dairy Ashford
Sugar Land, TX 77478
281-494-2516

WEBSITE
www.netl.doe.gov

CUSTOMER SERVICE
1-800-553-7681