netlognews

NETL's R&D newsletter

July 2013, Issue 30

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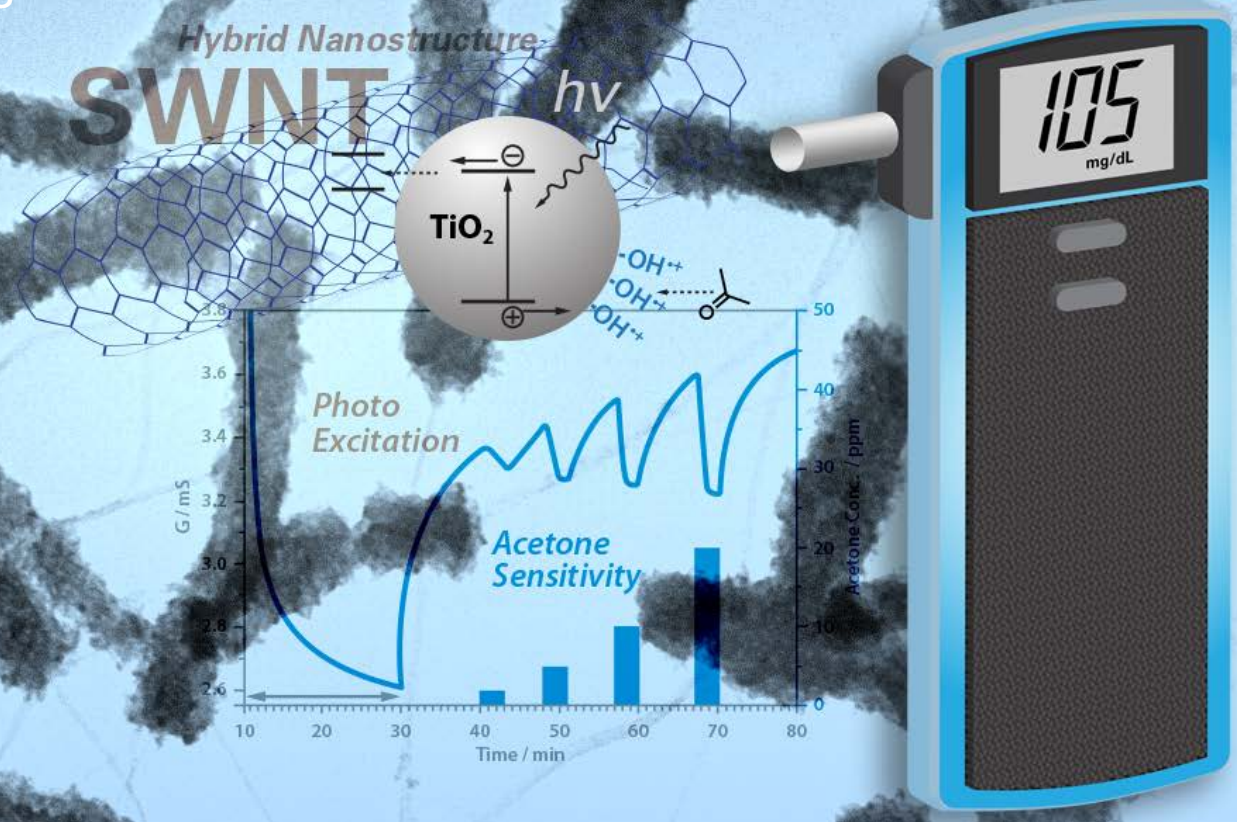

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Cover image: Illustration of carbon nanotubes and theoretical breathalyzer with photomicrograph of "titanium dioxide on a stick". *(photomicrograph image courtesy of the University of Pittsburgh)*

netlognews

newlognews is a quarterly newsletter highlighting 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.

National Energy Technology Laboratory metallurgist Dr. Paul Jablonski (far right), was named a finalist for a Partnership for Public Service Samuel J. Heyman Service to America Medal.

NETL Scientist Named Finalist for Service to America Medal

—In May 2013, NETL metallurgist Dr. Paul Jablonski was named a finalist for a Partnership for Public Service *Samuel J. Heyman Service to America Medal* – known as the *Sammies* – during a congressional breakfast ceremony in Washington, DC. The annual awards pay tribute to federal employees whose work advances the health, safety, and well-being of Americans. Medal recipients will be announced on October 3, 2013, at the Andrew Mellon Auditorium in Washington, D.C.

Dr. Jablonski is one of eight finalists – out of more than 300 nominees – for the prestigious *Science and Environment Medal* in recognition of his leading role in developing and fabricating a novel platinum-chromium alloy for use in new, state-of-the-art coronary stents. These stents are now being sold worldwide by the Boston Scientific Corporation.

Working with NETL colleagues Paul Turner and Ed Argetsinger, as well as scientists from Boston Scientific, Dr. Jablonski developed an alloy that is more visible in X-rays than traditional coronary stents and makes the new stents more resistant to corrosion and more flexible than conventional stents. These advances have led to improved clinical outcomes, better long-term prognosis for patients, and reduced healthcare costs.

Dr. Jablonski has had a distinguished career, authoring or co-authoring more than 65 peer-reviewed publications and collecting four patents. His numerous awards include three

R&D 100 Awards, a Secretary of Energy Achievement Award, and five Federal Laboratory Consortium Awards for Excellence in Technology Transfer – including the Consortium's award he and the NETL team received last year for their work on the new coronary stent alloy.

In June 2013, he was awarded the Arthur S. Flemming award presented by the George Washington University recognizing outstanding and meritorious achievements in working for the federal government.

In addition to his professional accomplishments, Dr. Jablonski is also known for his commitment to helping others. Always willing to share his knowledge and experience, he is a mentor to young people interested in pursuing a career in materials science and engineering. He is also active in charitable work in his community.

New Breathalyzer Offers the Potential for Non-invasive Diabetes Monitoring

—NETL researchers and their Regional University Alliance (NETL-RUA) colleagues have developed a new hybrid nanostructure material that could be used to develop a breathalyzer for self-monitoring diabetes. In this application, the NETL-RUA material could offer millions of diabetics an alternative non-invasive testing solution.

NETL-RUA researchers discovered that by bolstering titanium dioxide with carbon nanotubes (CNTs), they could produce an electrical semiconductor that acts as a sensor for the presence of acetone. Compared to non-diabetics, the acetone concentration in a diabetic's breath is much higher, producing a fruity aroma when glucose levels are high. Detecting gaseous components and condensates found in breath is challenging, and the new nanostructure-based breathalyzer would detect acetone at parts-per-million levels.

CNTs are highly conductive. Titanium dioxide is highly refractive and highly absorbent to UV rays. The resulting hybrid nanostructure exhibits unique behavior in response to UV illumination and subsequent exposure to acetone. When light activates the sensor to produce an electrical charge, the hybrid nanomaterial shows ultrahigh acetone sensitivity and a much lower detection limit.

CNT-based sensors might provide a cheaper and non-invasive testing method compared to the expensive, inconvenient blood tests diabetics currently rely on to monitor their glucose levels. Additionally, CNT-based sensors are extremely small and consume little power.

The NETL-RUA team-Alexander Star, principal investigator and an associate professor of chemistry at University of Pittsburgh; Dan Sorescu, a research physicist at NETL; and Mengning Ding,

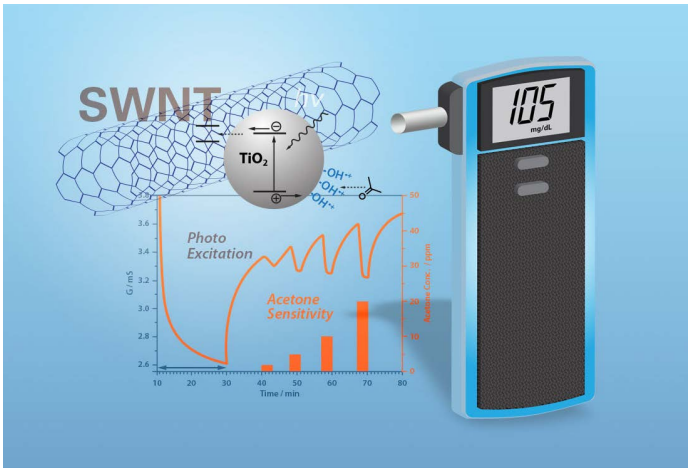


Illustration of the carbon nanotube-TiO_2 hybrid nanostructure to be used in a breathalyzer device.

a Pitt graduate student in chemistry-are now developing a prototype sensor. Successful clinical tests on human breath samples could mean a game–changing medical technology is on the way.

The findings of the NETL-RUA team are described in the paper "Photoinduced Charge Transfer and Acetone Sensitivity of Single-Walled Carbon Nanotube-Titanium Dioxide Hybrids," which was published recently in the *Journal of the American Chemical Society*.

Contact: Dan Sorescu, 412-386-4827

Photo taken inside a vacuum arc remelting furnace.

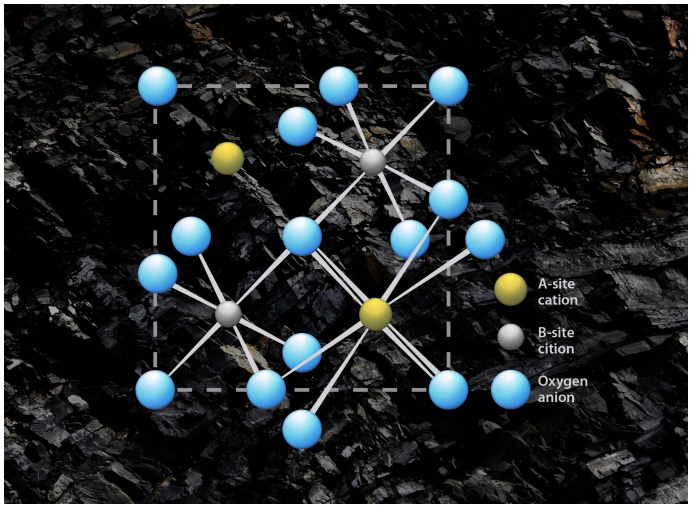
Database to Aid Advanced Alloy Processing—NETL's Paul Jablonski and Professor Zi-Kui Liu of the Materials Science and Engineering department at the Pennsylvania State University are developing a new CALPHAD (calculation of phase diagram) modeling thermodynamic database to aid in slag formulation for electro-slag remelting (ESR). The first version is now complete and includes the elements aluminum, calcium, chromium, fluorine, iron, magnesium, manganese, nickel, oxygen, silicon, and titanium. Assessed systems include binary, ternary, and oxide systems.

Electro-slag remelting is a manufacturing process employed in the production of advanced high-temperature steels and nickel superalloys for mission-critical applications including thermal power stations, nuclear power plants, aircraft, and military technologies. The process is used to refine and purify the chemistry of alloy ingots and is a critical step in the production of high-performance alloys. The slag plays a critical role in the ESR process, which uses an as-cast vacuum induction melted alloy ingot as a consumable electrode. An electric current is passed through the electrode into an engineered slag, which gradually melts the tip of the electrode. As the electrode melts, drops of molten metal descend through the slag to the mold, where they slowly freeze to form the new ESR ingot from the bottom up. Impurities are cleaned from the molten alloy by chemically reacting with the slag and/or floating with it to the top. The resultant ESR ingot is of the high chemical purity necessary for mission-critical components.

A better understanding of the slag is needed to produce the desired ingot chemistry (especially regarding trace elements, which can be either detrimental or beneficial) and ingot structure. This understanding and control of the slag has the potential to provide higher-quality ESR melted materials, which will be at the core of the fossil energy power plants of the future, such as advanced-ultrasupercritical (A-USC) coal-fired steam plants. The new database provides the foundation for NETL-RUA work on alloys, slag chemistries, and alloy-slag interactions. The next step in the development of the database is to establish and incorporate slag physical properties such as thermal and electrical conductivities, density, viscosity, and variations in temperature and chemistry. NETL-RUA researchers plan to use this database to optimize the re-melt processing of steam turbine rotor alloys for A-USC plants.

Contact: Paul Jablonski, 541-967-5982

NETL Catalyst Produces Winner in Shale Gas Innovation Contest—The Shale Gas Innovation & Commercialization Center (SGICC) selected Pyrochem Catalyst Company (PCC) a winner in this year's Innovation Contest. Contest winners receive $25,000 in seed capital to accelerate shale gas-related technologies toward commercialization. PCC is a Pittsburgh-based startup company, the first to be based on NETL-licensed technologies.



The η2 and η1-CT structures of the acetate-CO_2 complex.

Pyrochlore-type catalysts have proven to be effective catalysts for the reforming of a variety of hydrocarbon fuels into hydrogen-rich synthesis gas for fuel cells as well as refinery applications. Pyrochlore-type oxide compounds can be customized to increase selectivity and conversion by partial substitutions of catalytically active metals into the oxide lattice. With these metals well dispersed and locked into place in the crystal structure, metal sintering, which typically occurs on supported catalysts used in reforming reactions, and deactivation by sulfur and carbon are greatly reduced. The NETL collaboration that developed novel pyrochlore catalysts for reforming hydrocarbon fuels was recognized with the 2012 Research Collaboration Award from the Council for Chemical Research, a nonprofit organization dedicated to advancing research in chemistry, chemical engineering, and related disciplines.

Contacts: Dushyant Shekhawat, 304-285-4634 and David Berry, 304-285-4430

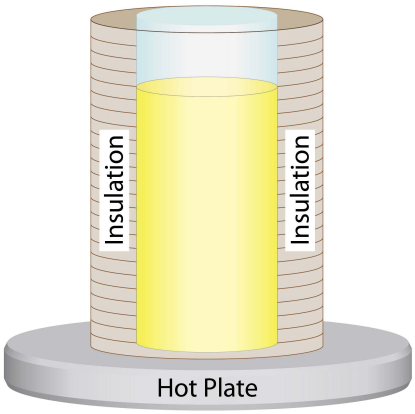


Illustration of the experiment on Al-slurry ignition using a hot plate.

NETL Research Highlights Potential Safety Concern of Nano-sized Aluminum Particles

—Amid concerns about the emissions of greenhouse gases associated with the use of fossil fuels for industrial applications and electricity production, efforts have been made to search for more alternative eco-friendly fuel sources. Aluminum and aluminum-based metals, therefore, have been recognized as the most promising alternative source because aluminum is the most abundant metal in earth's crust, can be fully recycled, and is lightweight. Aluminum reacts with water and produces heat, hydrogen, and eco-friendly aluminum oxides, which do not stick to the combustor and can be easily collected and widely used in alumina production, water treatment, paper making, and fire inhibition. Aluminum oxides can also be recycled back into usable fuel by heating and burning them using carbon monoxide, creating carbon dioxide. In this process, CO_2 is the only gaseous product so it can be removed easily, which greatly facilitates desirable carbon sequestration. The reactivity of aluminum-water slurries at low temperature can pose a significant safety concern for their storage and handling.

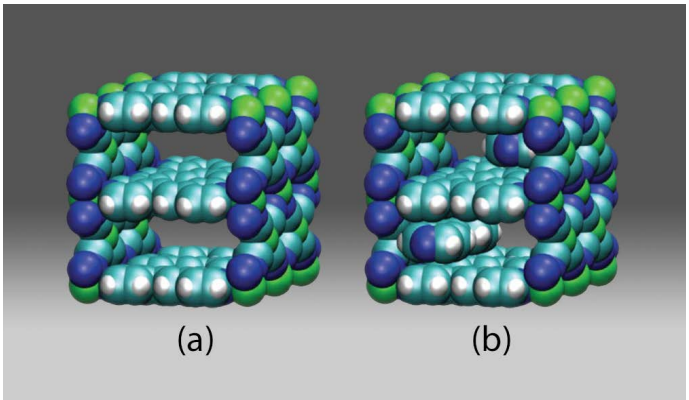
Experiments exploring the spontaneous ignition of Al/water slurries containing low aluminum weight fractions (17 percent and 27 percent) were conducted at low temperatures to compare the reactivity of nano-dispersed Al to large-particle samples.

The results showed that nano-Al/water slurry ignition occurred due to the reaction between Al and water even in the absence of air. Although Al/water slurry ignition of large Al particles does not occur below a temperature of about 321 K, the nano-particle slurry reacted at a temperature as low as 303 K, and the process could develop sufficient heat for the slurry to sustain its temperature rise until ignition occurred. The ability of the slurry to react at the low temperatures observed here can pose a significant safety concern in terms of slurry storage and handling. The study was published in *Applied Energy* (2013, 101, 567-571).

Contact: Phuoc Tran, 412-386-6024

NETL and NIST Collaborate to Study CO_2 Capture Sorbents that "Breathe"

—Researchers at NETL recently developed a new sorbent commonly called "nickel bpene"-that takes up significantly more CO_2 than conventional sorbents do. That alone is enough to make nickel bpene intriguing, but it is not the sorbent's most astonishing attribute. What sets it apart is its breathing-like behavior. Its pores open as they "inhale" CO_2 and close as they "exhale" it. The sorbent isn't actually breathing, of course, but the changes its pores undergo in the presence of CO_2 are curious nonetheless. Because nickel bpene is so good at isolating CO_2 , it shows enormous potential as a carbon-capture material.

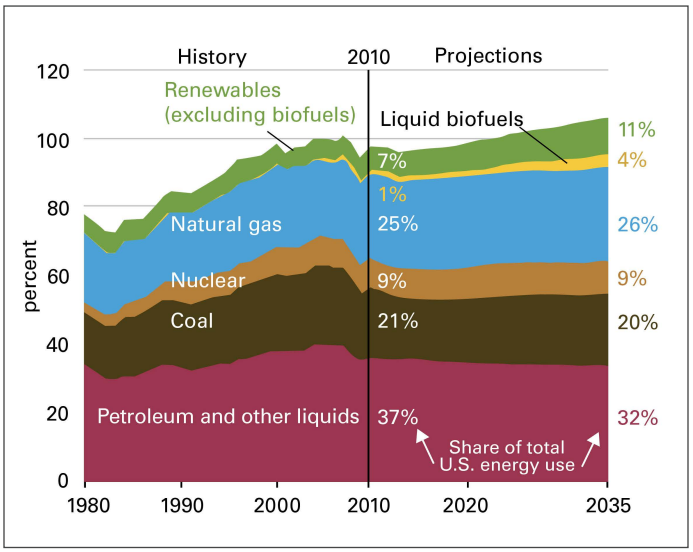


Molecular structure of Ni(bpene)[Ni(CN)4] (without solvent), with van der Waals exclusion volume of all atoms16 shown by colored spheres. Atomic positions were obtained via the crystallographic information from this work. (a) Structure without free bpene ligands. (b) Structure with free bpene ligands. Color codes for atoms: cyan, C; blue, N; white, H; green, Ni.

To get nickel bpene to divulge its secrets, researchers at NETL synthesized large, high-quality crystals of it so they could investigate the crystals' structure. "To solve structures, size is one issue--you need larger crystals--but quality of the crystal comes into play, so you need high-quality crystals," explains Dr. Christopher Matranga, a research chemist at NETL, who was on the research team. To address this issue, Dr. Jeffrey Culp, a researcher with URS Corporation (URS) set out to develop new synthetic approaches to make larger, higher-quality crystals. "We have made these crystals in the past, but they were not large enough or crystalline enough to be useful for determining the positions of atoms in the material," says Culp.

Because of the research team's efforts, NETL now has a map of every atom in the sorbent's pore network. This information is the most critical starting point for understanding how CO_2 interacts with the sorbent and for developing computational models, which can predict performance in power-plant applications. NETL worked with both the National Institute for Standards and Technology and with URS, an NETL-Regional University Alliance member organization on this research project. Being able to leverage the knowledge of scientists across agencies made it easier to examine the problem from several angles and increased the fruitfulness of the research. This research was captured in an article in *CrystEngComm*, a journal published by the Royal Society for Chemistry (2013, 15, 4684-4693). More importantly, it may lead to a highly efficient, cost-effective method to slash CO_2 emissions.

Contacts: Jeffrey Culp, 412-386-5393 and Christopher Matranga, 412-386-4114



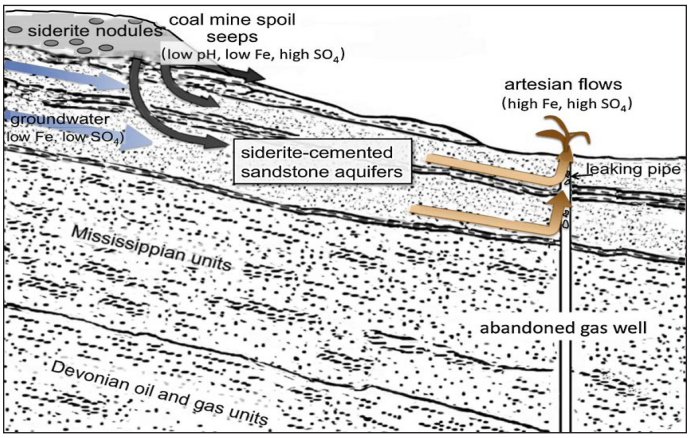
The Energy Information Administration is projecting a steady increase in U.S. demand for energy through 2035. An international increase is also expected.

National Academy of Sciences Publicizes Findings on Energy and Mining Workforce

—In a report produced in cooperation with NETL, a committee of experts selected by the National Academy of Sciences summarizes available data on the current and projected future workforce for the U.S. energy and mining industries—including oil, natural gas, coal, nuclear, solar, wind, geothermal, carbon capture utilization and storage, and nonfuel mineral mining. The

data from this report, *Emerging Workforce Trends in the U.S. Energy and Mining Industries: A Call to Action*, indicate a bright present and future for well-paying energy and mining jobs. Demand for workers at all levels in these industries will remain strong for the foreseeable future because of projected industry growth and the pending retirement of a large number of experienced workers. The report also addresses challenges in meeting that demand, recommending several improvements to the U.S. education system that would make it more oriented toward science, technology, engineering, and math, yet responsive to ever-expanding industry needs. The report in brief is also available.

Contact: Steven M. Seachman, 304-285-5448



Schematic hydrogeologic cross-section (modified from Merritt and Emrich (1970) and Hedin et al. (2005)) illustrating one conceptual model of the generation of the artesian gas well discharges. Acidic, sulfate-rich water associated with coal mine spoil (dark gray arrows) infiltrates into shallow sandstone aquifers, dissolving siderite cement and releasing iron. The contaminated waters enter deteriorating wells and are transported to the surface via artesian flow.

Study Attributes Water Contamination in Abandoned Gas Wells to Coal Mine Drainage

—Isotopic and geochemical analyses indicate that artesian discharges of water with high total dissolved solids from a series of gas wells in western Pennsylvania result from the infiltration of acidic, low iron (less than 10 milligrams per liter) coal mine drainage into shallow, sandstone aquifers cemented with siderite (a mineral composed of iron carbonate). The acidity promotes dissolution of the carbonate, and metal- and sulfate-contaminated waters rise to the surface through compromised abandoned gas well casings.

Strontium isotope mixing models suggest that neither upward migration of oil and gas brines from Devonian reservoirs associated with the wells nor dissolution of the abundant nodular siderite present in the mine spoil through which recharge water percolates contribute significantly to the artesian gas well discharges. Natural strontium isotope composition can be a sensitive tool for characterizing complex groundwater interactions and can be used to distinguish between inputs from deep and shallow contamination sources, as well as between groundwater and mineralogically similar but stratigraphically distinct rock units.

These findings have particular relevance for regions such as the Appalachian Basin, where a legacy of coal, oil, and gas exploration is coupled with ongoing and future natural gas drilling into deep reservoirs. Details of the NETL study, conducted jointly with the University of Pittsburgh and others, appeared in the April 2013 issue of the Elsevier publication *Applied Geochemistry*. (Vol. 31 (2013), pp. 109-118).

Contact: Hank Edenborn, 412-386-6539

Dr. Margaret Ziomek-Moroz holding her NACE International award.

NETL Scientist Receives NACE International Award

—NETL has a strong record in advancing corrosion science through the efforts of its team of corrosion scientists. NACE International, The Corrosion Society, recently recognized Dr. Margaret Ziomek-Moroz for having made a significant and lasting contribution in corrosion science and engineering. Dr. Ziomek-Moroz received a 2013 NACE International Technical Achievement Award for the breadth of her contributions to the field of corrosion science, both as an educator and a researcher.

For nearly a decade, Dr. Ziomek-Moroz was a professor at the Oregon Graduate Institute of Science and Technology. Her mentoring work guided students into the field of corrosion, where their research earned recognition through NACE student awards. Dr. Ziomek-Moroz also has been a role model for middle and high school students interested in math, science, and engineering through her participation in the U.S. Department of Energy-sponsored Science Bowl and in DaVinci Days, Oregon's premier arts and science festival.

Dr. Ziomek-Moroz has made advancements in a wide variety of areas. Her contributions include the development of thermal spray zinc and titanium used for the cathodic protection of coastal bridges, the creation of materials for solid oxide fuel cell interconnects, and the electrochemical machining of alloys.

Contact: Margaret Ziomek-Moroz, 541-967-5943

NETL Researcher Receives Award from the US Department of Justice

—Dr. Barbara Kutchko has received a Certificate of Commendation for outstanding performance and invaluable assistance in support of the activities of the Environmental and Natural Resources Division of the U.S. Department of Justice. The award is in recognition of the rapid turnaround and expert interpretation of data obtained from samples associated with the Macondo Well uncontrolled release event in the Gulf of Mexico in 2010.

Contact: Barbara Kutchko, 412-386-5149

Models Supplied to Support Future Oxy-Combustion Demonstration at Full Scale

—NETL researchers have turned over models developed with GE-GateCycle© software to Jupiter Oxygen Corporation (Jupiter), completing a decade-long partnership in exploring how to use the high-temperature flames produced when oxy-fuel combustion occurs with low rates of flue gas recycle. The high-temperature approach introduces oxygen content as a new degree of freedom in designing boilers for systems that can potentially deliver power at lower cost than other carbon capture technologies. Greenfield boilers designed for high-temperature could maintain optimum heat flux with less heat transfer surface, reducing capital cost. These smaller boilers could also achieve lower operating costs through modularity of design and greater recovery of energy from combustion products using, for example, Jupiter-patented IPR® (integrated pollutant removal) technology co-invented with NETL.

Analysis of Jupiter's oxy-combustion data allowed NETL researchers to determine that converting coal-fired power plants to natural gas is greatly facilitated by the improved heat transfer balancing afforded with oxy-natural gas (ONG) at high temperatures. The models showed that transitioning to ONG could lead to rapid reduction in carbon emissions either with full-scale retrofits or new designs. With the NETL models now in hand, JOX and partners can choose the design options that will best demonstrate low-recycle oxy-fuel combustion at full scale.

Contact: Tom Ochs, 541-990-5443

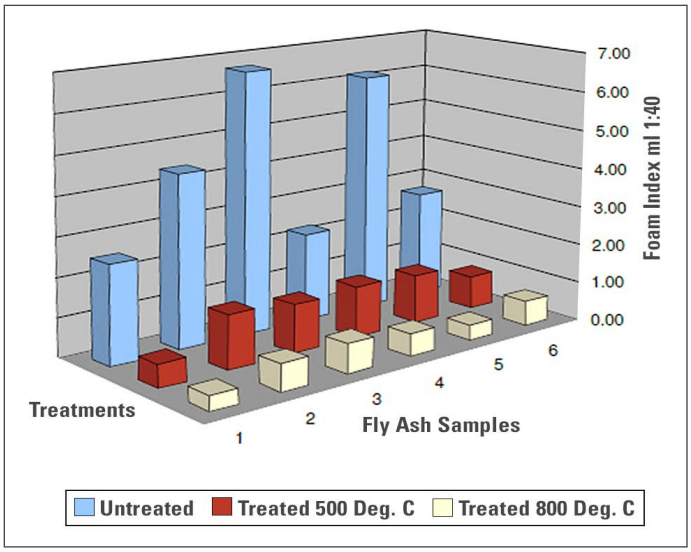


Figure showing decrease in foam index (AEA requirement) for different fly ash samples upon thermal treatment in 10% oxygen (balance argon) for two different temperatures.

NETL and Waynesburg University Researchers Awarded Patent on Fly Ash Carbon Passivation

—Coal combustion fly ash is often used commercially as a replacement for some of the Portland cement in concrete products. Some fly ash is not suitable for concrete because it requires excessive amounts of air entrainment agent (AEA) surfactants owing to the fly ash chemical composition, including high carbon content, which inactivate the AEA's through adsorption or chemical reaction. AEAs are typically added to increase workability of concrete mixtures and enhance durability of the final products to freeze-thaw cycles.

John Baltrus, a research chemist in NETL's Chemistry and Surface Science Division, along with Robert LaCount and Douglas Kern of Waynesburg University, were recently awarded a U.S. Patent #8,440,015 for their method called "Fly ash carbon passivation."

The patent describes a thermal method to passivate the carbon and/or other components in fly ash while retaining the carbon in the fly ash. Such passivation, which involves heating the fly ash to between 400 °C and 800 °C under inert gas containing up to 10 percent oxygen, results in sharply decreased amounts of surfactants that need to be added to the fly ash despite the fact that most of the carbon remains in the fly ash.

The patented method reduces the temperature requirement and carbon burnout, both resulting in lower greenhouse gas emissions. The patent culminates a cooperative project that led to coauthored peer-reviewed journal articles on the subject by the inventors.

Contact: John P. Baltrus, 412-386-4570

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2.	Wells, Arthur W.; Diehl, J. Rodney; Strazisar, Brian R.; Wilson, Thomas H.; Stanko, Dennis C. May 2013. Atmospheric and Soil-Gas Monitoring for Surface Leakage at the San Juan Basin CO2 Pilot Test Site at Pump Canyon, New Mexico, using Perfluorocarbon Tracers, CO_2 Soil-Gas Flux and Soil-Gas Hydrocarbons, *Intl. J. Greenhouse Gas Control*, 14, 227-238.
3.	Kutchko, Barbara G.; Goodman, Angela L., et al. May 2013. Characterization of Coal Before and After Supercritical CO_2 Exposure via Feature Relocation Using Field-Emission Scanning Electron Microscopy, *Fuel,* 107, 777-786.
4.	Mao, James X.; Lee, Anita S.; Kitchin, John R., et al. April 24, 2013. Interactions in 1-Ethyl-3-Methyl Imidazolium Tetracyanoborate Ion Pair: Spectroscopic and Density Functional Study, *J. Molecular Structure*, 1038 , 12-18.
5.	Chapman, Elizabeth C.; Capo, Rosemary C,; et al. April 2013. Strontium Isotope Quantification of Siderite, Brine and Acid Mine Drainage Contributions to Abandoned Gas Well Discharges in the Appalachian Plateau, *Applied Geochemistry*, 31, 109-118
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8.	Rupp, Erik C.; Granite, Evan J.; Stanko, Dennis C. June 2013. Laboratory Scale Studies of Pd/gamma-Al2O3 Sorbents for the Removal of Trace Contaminants From Coal-Derived Fuel Gas at Elevated Temperatures, *Fuel*, 108, 131-136.
9.	Siriwardane, Ranjani; Tian, Hanjing; Simonyi, Thomas; et al. June 2013. Synergetic effects of mixed copper-iron oxides oxygen carriers in chemical looping combustion, *Fuel*, 108, 319-333.
10.	Brubaker, Tonya M.; Stewart, Brian W.; Capo, Rosemary C.; et al. May 2013. Coal Fly Ash Interaction With Environmental Fluids: Geochemical and Strontium Isotope Results From Combined Column and Batch Leaching Experiments, *Applied* Geochemistry, 32, SI, 184-194.
11.	Romanov, Vyacheslav N. May 2013. Evidence of irreversible CO_2 intercalation in montmorillonite, Intl. J. *Greenhouse Gas Control,* 14, 220-226.
12.	Mhatre, B. S.; Pushkarev, V.; Holsclaw, B.; et al. April 18, 2013. A Window on Surface Explosions: Tartaric Acid on Cu(110), J. *Phys. Chem. C*, 117, 15, 7577-7588.
13.	Kauffman, Douglas R.; Alfonso, Dominic; Matranga, Christopher; et al. April 18, 2013. A Quantum Alloy: The Ligand-Protected Au25-xAgx(SR)(18) Cluster, J. *Phys. Chem. C*, 117, 15, 7914-7923.

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15.	Jablonski, Paul D.; Sears, John S. April 15, 2013. The Impact of Alloy Chemistry on the Formation of a Silicon-rich Subscale on Two Classes of Ferritic Steels, J. *Power Sources*, 228, 141-150.
16.	Allen, Jesse J.; Schneider, Yanika; Kail, Brian W.; et al. April 11, 2013. Nuclear Spin Relaxation and Molecular Interactions of a Novel Triazolium-Based Ionic Liquid, J. *Phys. Chem. B*, 117 (14) 3877-3883.
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25.	Ding, Mengning; Star, Alexander. March 27, 2013. Synthesis of One-Dimensional SiC Nanostructures from a Glassy Buckypaper, *ACS Applied Materials & Interfaces*, 5 (6) 1928-1936.
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Patents Issued This Quarter

1.	A process for the mixing of heavy solid particulate matter in a lighter liquid carrier fluid using an inverted pulsed jet mixing apparatus, John G. VanOsdol, **8,469,583**, issued June 25, 2013.
2.	Process for CO_2 Capture from $Mg(OH)_2$ Sorbent at High Pressure and Moderate Temperature Gas Streams, Ranjani V. Siriwardane and Robert Stevens, **8,470,276**, issued May 14, 2013.
3.	Fly Ash Carbon Passivation. Robert B. LaCount, John P. Baltrus, and Douglas G. Kern, **8,440,015**, issued May 13, 2013.
4.	Nanocomposite Thin Films Consisting of Plasmonic Sensing Materials and Non-Catalytic High Temperature Stable Dielectric Materials for High Temperature Optical Gas Sensing, Thomas Brown and Paul Ohodnicki, Jr. , **8,411,275**, issued April 2, 2013.

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