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Research news

December 2014, Issue 3

FEATURE STORY:

ORD's Catalysis Expertise is Key to a Cleaner Energy Future

page 3

the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

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Research news
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ORD's Catalysis Expertise is Key to a Cleaner Energy Future

NETL's Dushyant Shekhawat and Bill Grimes are preparing the Catalyst Screening Unit in NETL's Reactor Laboratory for diesel reforming runs.

Did you know that catalysts can be used to convert carbon dioxide (CO_2) into a useable fuel? Or that catalysts can use clean, free sunlight to drive CO_2 conversion to useful chemicals? The Office of Research and Development (ORD) is harnessing the power of catalysts to make energy production cleaner and more efficient, and to find effective ways to utilize the waste products of energy production (like CO_2): both priorities of U.S. Department of Energy research.

By converting hydrocarbons and CO_2 to useful products, catalysts can enable a carbon-neutral cycle for fossil fuels utilization, making coal and natural gas viable clean energy choices for the nation and the world. Custom-designed catalysts made by ORD researchers can promote the photocatalytic reduction of CO_2 or quickly convert heavy hydrocarbons into synthesis gas for fuel cells. And these are just a few examples.

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Research News is a monthly publication from the National Energy Technology Laboratory's Office of Research and Development. We focus on the exciting research done at NETL by our scientists and collaborators.

Research News welcomes your comments, questions, and suggestions. Call us at **541-967-5966**.

Cover image
Researchers working in the Surface Science laboratory in Pittsburgh, Pa.

NETL's unique expertise and capabilities are solving many challenges in the development of new catalysts. ORD researchers use a variety of techniques, including computational design and atomic-level synthesis, to create catalysts that enable, enhance, or prevent chemical reactions. Collaboration between expert computational and experimental scientists and engineers enhances ORD's ability to create new fit-for-purpose catalysts. Researchers study and design catalysts at the atomic scale, investigate their performance at the bench scale, and later demonstrate at the industrial scale as they move toward commercialization. The result is the development of advanced catalysts that reform fuels for use in advanced clean energy systems, and mitigate CO_2 emissions by converting this greenhouse gas into useful chemicals and fuels. See sidebar (page 4) for more information about NETL's facilities for catalysis development.

ORD catalyst research encompasses a broad range of technology innovation, from design to commercialization. Two examples illustrating this research spectrum are NETL's gold nanocatalyst and its pyrochlore catalyst.

To design the patent-pending gold nanocatalyst, ORD scientists collaborated with researchers from West Virginia University (WVU). The resulting catalyst converts visible light into heat energy, which can then be used to drive the transformation of CO_2 into carbon monoxide (CO) or methane (CH_4), either of which can then be used for fuel or chemical production.

The gold particles must be nanosized—about 100,000 times smaller than the diameter of a human hair—to efficiently convert visible light to heat. When exposed to visible light, the gold nanoparticles—paired with zinc oxide (ZnO) nanoparticles as the catalytically active substrate—cause the system's temperature to rise. The heat and ZnO, in turn, change CO_2 into useful chemicals such as CO and CH4. Controlling the intensity of the light allows CO and CH_4 to be produced in different ratios.

Not only does use of the gold nanocatalyst make it possible to use the CO_2 emitted during energy production, but it can also lead to valuable products that can offset the cost of carbon capture technologies.

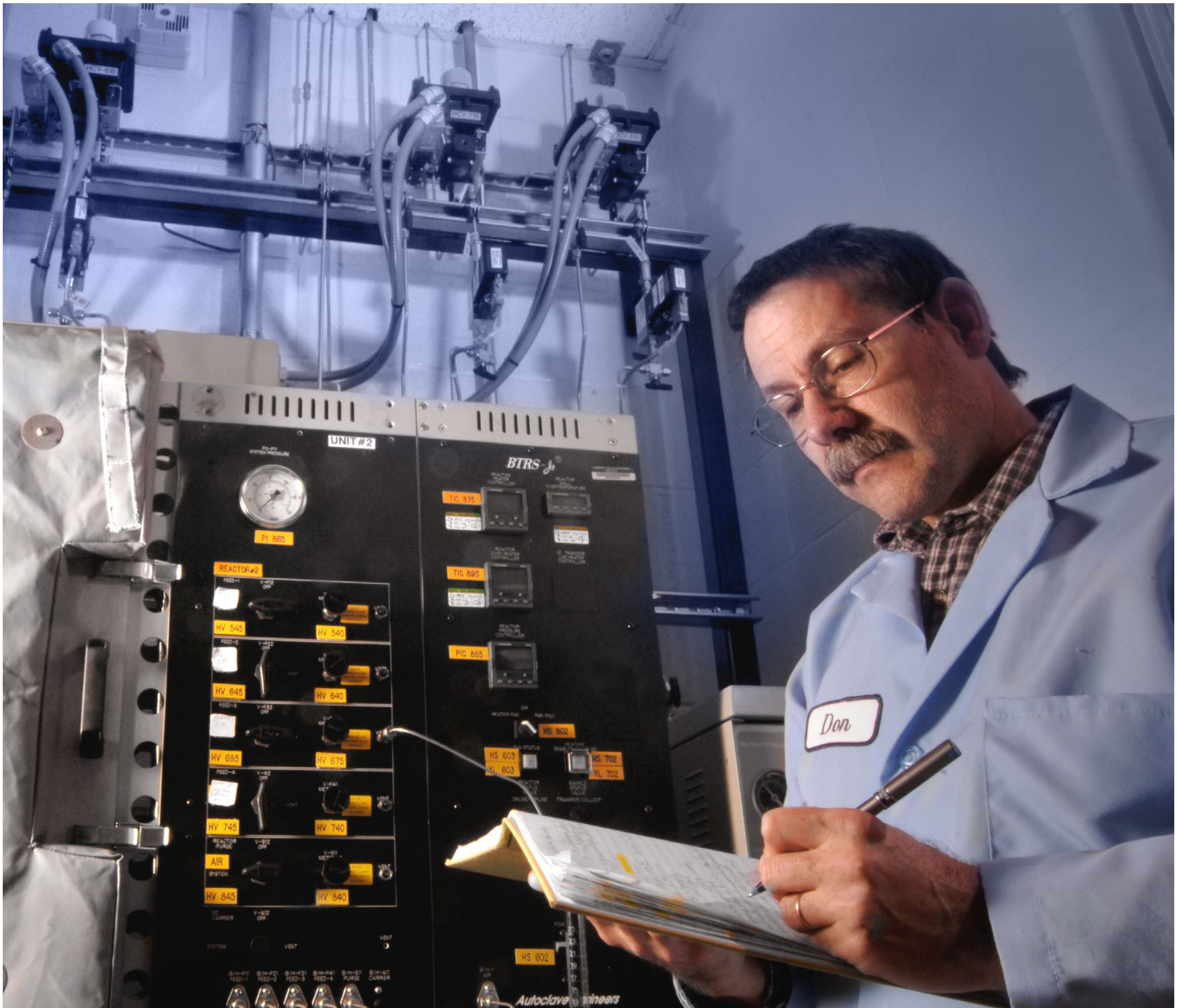
NETL researchers Dan Haynes (left) and Mark Smith synthesize the NETL pyrochlore catalyst.

ORD's award-winning pyrochlore catalyst can improve air quality by reducing emissions. For example, the catalyst can be used to convert hydrocarbon fuels, such as shale gas and diesel, into clean-burning syngas—a transformation that has found application in the long-haul trucking industry. In this case, the catalyst provides syngas to fuel solid oxide fuel cells (SOFCs) that run a truck's auxiliary power unit (APU). The APU powers HVAC and lighting while the truck is parked. Relying on the APU means truckers no longer need to leave the engine idling to power these services.

The commercial value of the pycrochlore catalyst is evident, as its use can allow the trucking industry to comply with regulations while helping to reduce fuel costs. **Dr. Dave Berry**, director of ORD's Energy Process Innovation Division, led the team designing the catalyst. He explained that "the catalyst helps reduce fuel consumption, lower emissions, and extend engine life, all of which lead to overall cost reduction and environmental benefit." In addition to truck transport power, the pyrochlore catalyst can also be used to benefit military power applications, as well as to enable clean electricity generation for homes and businesses.

The pyrchlore catalyst's commercial viability has not gone unrealized. Following the initial research and development phase, and after establishing the performance benefit of the catalyst, NETL's technology transfer team searched for industry partners that could continue the research or market the technology for use in power plants or energy products. Pyrochem Catalyst Corporation (PCC), a startup company founded specifically for research and development on this fuel reforming technology, signed an exclusive licensing agreement with NETL in 2011. As a result of this partnership, the pyrochlore catalyst received a 2011 Federal Laboratory Consortium Award for Excellence in Technology Transfer. In 2013, the pyrochlore catalyst was recognized with an award for shale gas innovations from the Shale Gas Innovation & Commercialization Center. In 2014, PCC won a National Science Foundation grant to further develop a commercially attractive and innovative synthesis process for NETL's pyrochlore catalyst. Also in 2014, PCC made their first commercial sale of the catalyst for a defense application. PCC is evaluating and pursuing other relevant and viable markets as it continues development of the pyrochlore catalyst.

Contact: Dave Berry, Chris Matranga



*Researcher **Don Floyd** collects process data during a catalytic diesel fuel reforming experiment to generate hydrogen for fuel cells in the Fuels Processing Laboratory.*

Surface Science Lab

Because catalytic reactions almost always occur on a surface, studying the surfaces of materials and their properties is one of the keys to understanding how catalysts alter chemical reactions between materials.

The specialized instruments in NETL's Surface Science Laboratory allow researchers to investigate the chemical and physical interactions occurring at the atomic scale, to better understand how materials react when exposed to various substances. The Omicron Surface Analysis and Imaging System includes capabilities such as scanning tunneling microscopy and ion-scattering spectroscopy that allow researchers to view surface atoms and reveal the chemical and structural properties of a surface.

Instruments including x-ray photoelectron spectroscopy help researchers determine the speed at which chemical reactions occur on surfaces and study these reactions on the atomic level. Using techniques such as atomic force microscopy, researchers can manipulate and image surface molecules to understand how they react with the layers below.

CCSI
Carbon Capture Simulation Initiative

Programming Success

In the United States, power plants emit about 2.2 billion tons of CO_2 every year, roughly 40 percent of the nation's total emissions. Modernizing these plants to enable affordable CO_2 capture is crucial to reducing these numbers, and technological innovation is critical to overcoming these challenges. Moving technology from the laboratory to the real world takes time and costs money, and the very real risk of failure makes energy producers reluctant to adopt new technologies.

NETL's Carbon Capture Simulation Initiative (CCSI), an innovatively structured collaboration of national laboratories, universities, and industry, is developing tools that can help overcome these obstacles and hasten the commercialization of carbon capture technologies. CCSI uses these strategic partnerships to provide industry with an array of modeling and simulation tools dedicated to assessing and mitigating the risks associated with deploying carbon capture technologies. The initiative exploits core strengths throughout the Department of Energy (DOE) national laboratory system in modeling and simulation relevant to designing and optimizing pollution mitigation processes and improving integrated fossil-fuel powered electric generation plants.

The software resulting from this collaboration is called the CCSI Toolset, and comprises a suite of more than 30 computational tools and models. First released in 2012, these tools reduce the time needed to identify promising ideas, design and troubleshoot new systems, and more accurately represent the risk associated with scaling up a technology.

The CCSI Toolset is currently licensed to five industry partners—General Electric, Alstom, Phillips66, Babcock & Wilcox, and Chevron—with four more companies working to finalize agreements. Their input is what guides the future development of the project.

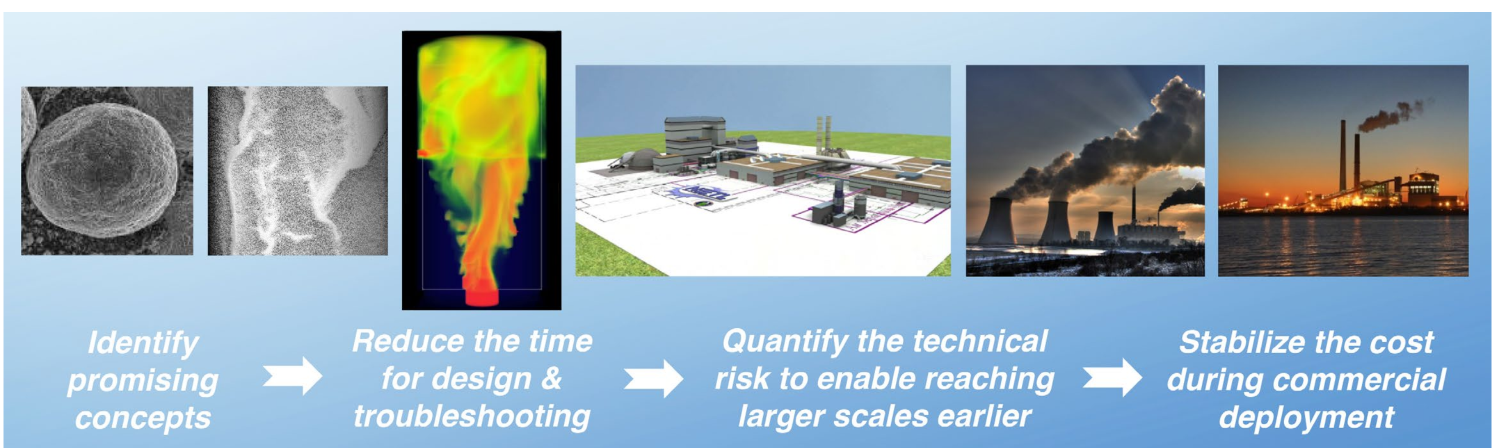
CCSI technical director **Dr. David Miller** finds interaction with industrial partners to be invaluable. "Industry feedback enables us to respond and design a release that enables users to more effectively utilize advanced computational capabilities to accelerate technology development," he said.

The latest version of the CCSI Toolset represents its third release, providing new capabilities, more streamlined workflows, and improved usability. Among other capabilities, the new release includes an integrated Framework for Optimization and Quantification of Uncertainty and Sensitivity (FOQUS), a tool that makes it possible to run hundreds of simulations in parallel to support large-scale optimization, uncertainty quantification, and the development of more computationally efficient surrogate models.

The CCSI Toolset stands to benefit more technologies than just carbon capture. As Chris Latham from Babcock & Wilcox, explained, "The Toolset will be broadly applicable to the development and scale-up of advanced energy conversion and emissions control systems."

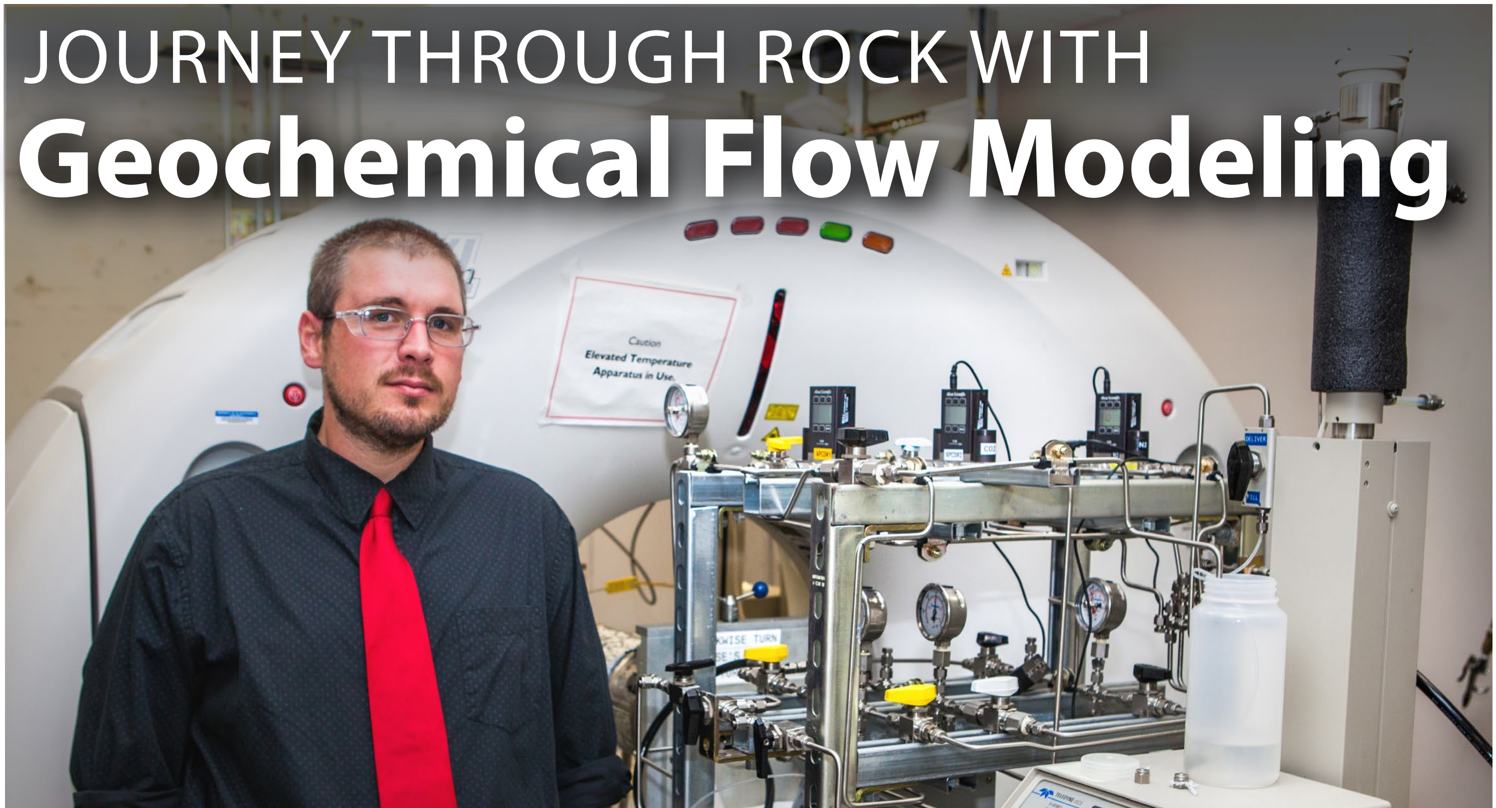
From CCSI's innovative structure, to its development of an adaptable and practical Toolset, the initiative is a powerful and ongoing technology transfer success story. The CCSI Toolset is helping meet a critical need, quickly and effectively taking carbon capture concepts from the laboratory to the real world.

Contact: David Miller



CCSI speeds up the development and deployment of carbon capture technologies.

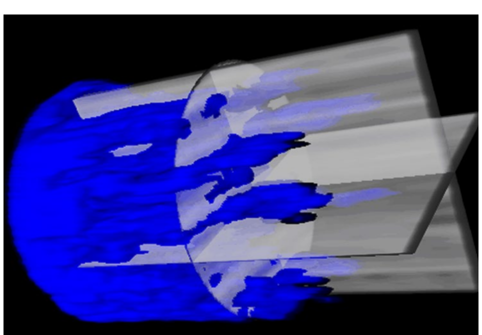
JOURNEY THROUGH ROCK WITH
Geochemical Flow Modeling



Dustin Crandall stands next to the Medical CT Scanner at the CT Imaging Facility.

Comparing rock layers within the Earth to sponges may seem strange, but in reality, rocks, like sponges, contain thousands of pores and small cracks that can act as pathways for fluids. ORD researchers are unlocking the mysteries about how these hidden pathways enable fluid motion, with the goal of maximizing geothermal power generation and improving underground storage of CO_2, resulting in cleaner, safer energy.

To understand the flow of fluids through rock, ORD researchers must be able to "see" inside the rocks, under the same conditions the rocks experience underground. ORD scientists accomplish this by using computed tomography (CT) scanners to analyze cores of rock drilled from the Earth. These samples are placed into specially designed containers that simulate the high-pressure and high-temperature conditions underground. Pumps inject fluids through the samples, and as they journey through the core sample, the CT scanner images the pathways they take through the rock, showing what happens underground.



CT-scanned image of CO_2 moving through a sandstone core.

As ORD researcher **Dr. Dustin Crandall** explained, the tests look at "real materials under real conditions," to understand what happens in the subsurface.

Researchers use the images created to validate and verify flow models, numerical models that describe the motion observed within the rock. But models only tell part of the story. As the scans illustrate how fluids move through rock, geochemical analysis answers how the fluid and rock interact. Minerals play a key role.

In active geothermal fields, water is injected into hot rocks to mine heat for geothermal power generation. When the injected water returns to the surface after its journey through the rock, it is not only hotter, but often is geochemically altered. By analyzing the composition of the water, researchers can determine how rocks in the subsurface interact with the fluids and understand the evolution of the fluid pathways over time.

The change in composition of the water is important to understanding how to maximize long-term geothermal field operation. If water returns to the surface enriched in dissolved calcite, for example, researchers know that the fractures are expanding as the fluid dissolves minerals surrounding the fractures and that the flow paths are becoming more permeable, ensuring a better flow through the rock.

In addition to the information it can provide about geothermal power generation, geochemical flow modeling also aids in understanding how carbon storage can be performed safely. It's important that the stored CO_2 permanently remains in the geologic formation. By understanding geochemical flow interactions, scientists can identify how CO_2 alters potential flow paths above storage reservoirs, and mitigation techniques can be developed to prevent CO_2 from escaping from the rock and into the atmosphere.

Read more about geochemical flow modeling here.

Contact: Dustin Crandall

NETL–University of Genoa Collaboration Creates Synergies in Advanced Power System Innovation

Only two places in the world—NETL and Italy's University of Genoa—host cyber-physical facilities for studying hybrid power systems that couple distinct technologies such as fuel cells and turbines. Now the two organizations have joined forces, so that energy researchers, students, and private-industry leaders around the world can gain a better understanding of how highly efficient, low-emission hybrid power systems function. The information flowing from this collaboration is enabling technologies that have the potential to double the power generation efficiency of coal and extend the service life of new fuel cells.

NETL's Hybrid Performance (HyPer) project facility and the University of Genoa's Hybrid System Emulator have complementary capabilities for developing control strategies for advanced power systems. Both use simulations and hardware components to study how coupled technologies interact. And both use a virtual fuel cell coupled with an actual pilot-scale gas turbine.

The combination approach allows the research to be conducted without destroying expensive fuel cells in the process. According to NETL Researcher **Dr. David Tucker**, it would have cost billions of dollars to date to conduct this research using actual fuel cells. The technique also yields detailed computational models of specific components as an alternative to modeling entire power systems.

NETL researchers use data from the HyPer facility to study operability—how a system responds to defined conditions, and how to control those responses. Meanwhile, University of Genoa researchers use data from both facilities to study performance and optimization. Researchers at Genoa address issues like how photovoltaics work with turbines and boilers.

But the collaboration goes beyond data and facilities. Tucker currently mentors three international students in the HyPer facility—including one from Genoa—and a postdoctoral researcher also from Genoa. The uniqueness of the NETL facility has attracted students from as far away as Malaysia and China, including **Farida Harun** and **Nana Zhou**. For **Paolo Pezzini** and **Valentina Zaccaria,** the NETL experience rounds out their University of Genoa education.

The collaboration, which has been ongoing for 8 years, has resulted in 12 joint publications, two doctoral graduates, and the exchange of two professors between Genoa and NETL research partner WVU. Experts from all over the world came to Morgantown, WV, in 2010 for the Low-Emission Advanced Power Research Workshop, where NETL researchers demonstrated the HyPer facility's hardware and, in coordination with Genoa researchers, ran simulations in real-time.

The technological advances resulting from this collaboration are providing global benefits. The combined NETL–Genoa effort is helping industry use technology to balance intermittent power sources, such as solar, with other sources on the grid. In addition, control strategies developed between NETL and the University of Genoa that mitigate degradation effects have succeeded in extending the life of fuel cells by 1,000 percent. "We've made a technology economically viable that wasn't an economical option before," said Tucker.

Contact: David Tucker

NETL's HyPer facility couples a physical pilot-scale gas turbine (shown here) with simulated fuel cells. From left: Paolo Pezzini, Valentina Zaccaria, David Tucker, Farida Harun, and Nana Zhou.

NETL's In-House Research Program:
Carbon Storage

About 40 percent of the United States' CO_2 emissions come from fossil-fueled power plants. This makes capturing the CO_2 released by power plants—and storing it underground—an important option for curbing anthropogenic CO_2 emissions. [Carbon capture and storage (CCS) technologies] can significantly reduce the volume of greenhouse gases we discharge. They can also help make the burning of fossil fuels more compatible with good environmental stewardship. NETL-ORD researchers are developing the science and technologies that make CCS safer and more cost-effective, with a focus on predicting the CO_2 storage capacity of geologic formations; understanding how CO_2 will interact with the formation once injected; and developing low-cost CO_2 utilization technologies. This year's research program includes the following key tasks:

- Improve reservoir characterization to ensure CO_2 storage permanence and predict storage capacity.
- Investigate characteristics of shale as CO_2 storage reservoirs and reservoir seals.
- Develop protocols and tools for new monitoring strategies for groundwater systems, including laser induced breakdown spectroscopy and isotope tracking.
- Develop methods for regional assessments of prospective storage resources.
- Advance geospatial data platforms, such as the National Carbon Sequestration Database and Geographic Information System (NATCARB) and Energy Data eXchange (EDX), to integrate public data and provide research tools for site characterization and resource assessments.
- Assess tools for monitoring CO_2 and pressure plumes at depth.
- Research new catalyst technologies for converting CO_2 into saleable chemicals.
- Evaluate ways to use and reuse CO_2—through feasibility studies, life-cycle analyses, and economic-benefit analyses—to guide future research.
- Assess the relationship between earthquakes and their possible triggers, such as CCS.

For more information on this research, contact Angela Goodman.

FUNDAMENTAL FUN

Basics of Catalysts

Catalysts work in a variety of ways, and there are many different types of catalysts. In general, catalysts work by forming an alternate reaction pathway. Reactant A reacts with the catalyst to form an intermediate product, which then reacts with Reactant B to form the final product. The reaction pathways that catalysts provide require less activation energy than the original reaction. As a result, catalysts accelerate chemical reactions. Adding the right catalyst to a set of chemicals increases the amount of product made in the reaction in a given amount of time, compared to an uncatalyzed reaction. As a bonus, the catalyst isn't used up in the reaction.

Speeding up chemical reactions makes processes more efficient and can reduce the amount of unwanted products. Catalysts can be used to reduce greenhouse gas emissions, including CO_2 and NOX.

We depend on many important catalytic processes, including—

- Fluid catalytic cracking, a process that converts heavy oils into fuels—such as gasoline and propane—and chemical feedstocks for producing plastics, cosmetics, and other goods.
- Treatment of automobile exhausts, which reduces CO, nitrogen oxide, hydrocarbons, and harmful, sulfur-based gas emissions.
- Polymerization, which produces adhesives, packaging, textile and industrial fibers, and electronic devices.

APPLAUSE

Patent Issued

Method of CO_2 Removal from a Gaseous Stream at Reduced Temperature; **Ranjani V. Siriwardane** (DOE/NETL); **George A. Richards** (DOE/NETL); **David A. Berry** (DOE/NETL); **James C. Fisher, II** (URS); 8888895, issued November 18, 2014.

License for NETL Intellectual Property

Issued to Michael Berry, non-exclusive license for US Patent Number 7,553,517, "Method of Applying a Cerium Diffusion Coating to a Metallic Alloy."

A recently released NETL technical report describes results of a field study that monitored a hydraulic fracturing operation in Greene County, PA. The study assessed upward fracture growth out of the target zone, and upward gas and fluid migration. Results indicated that under the conditions of this study, for this specific location, fracture growth ceased more than 5,000 feet below drinking water aquifers, and there was no detectable upward migration of gas or fluids from the hydraulically fractured Marcellus Shale.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An Evaluation of Fracture Growth and Gas/Fluid Migration as Horizontal Marcellus Shale Gas Wells are Hydraulically F…

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EXTRA! EXTRA!

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