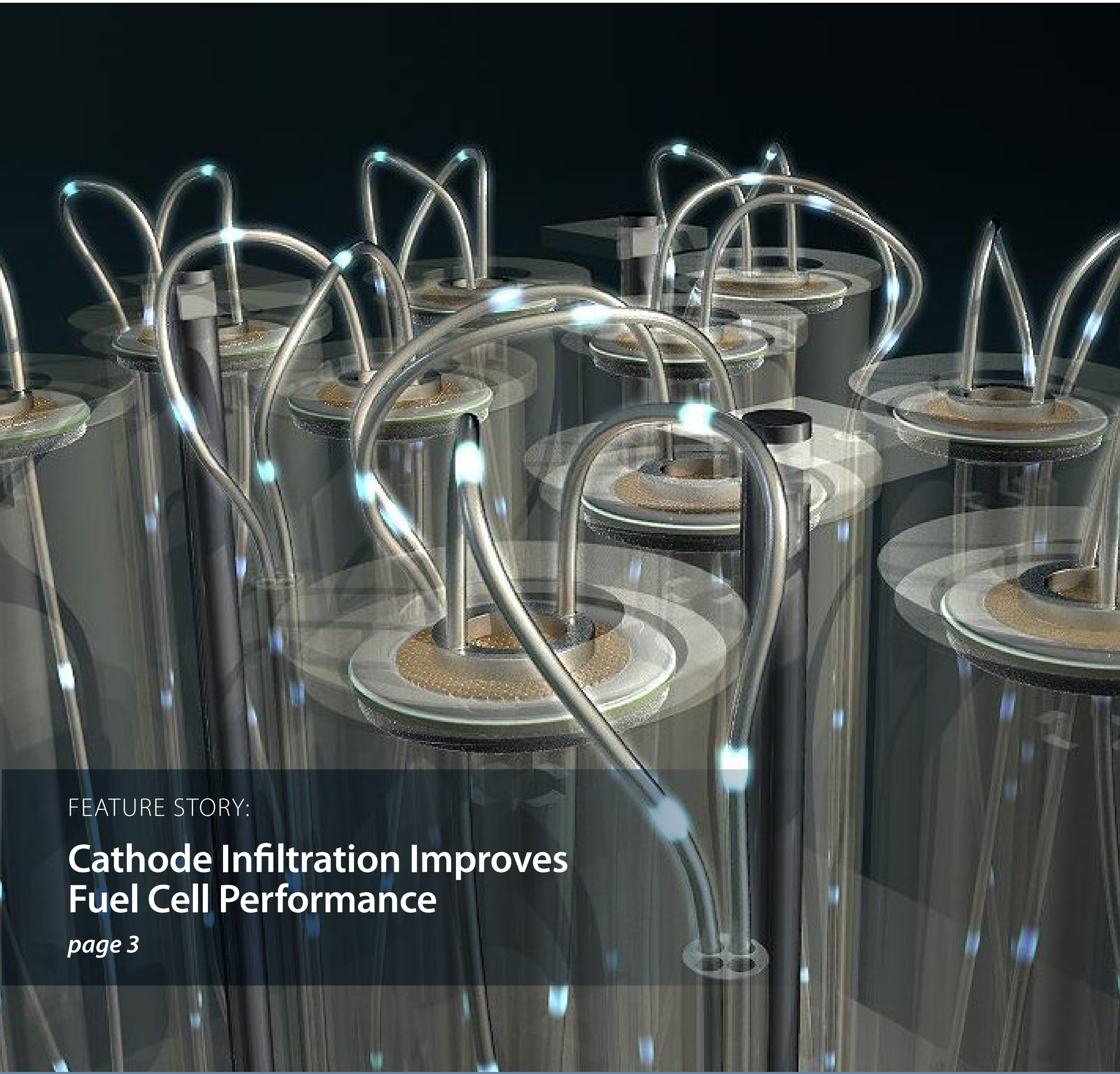
From NETL's Office of Research & Development

Research news

April 2015, Issue 7



FEATURE STORY:

Cathode Infiltration Improves Fuel Cell Performance

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the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

U.S. DEPARTMENT OF ENERGY

Research news
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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, cutting-edge research done at NETL by our scientists and collaborators to support the DOE Fossil Energy mission.

Research News welcomes your comments, questions, and suggestions.

NETL's In-House Research Competencies

The Office of Research and Development is committed to maintaining a knowledge base and laboratory facilities in support of the DOE Office of Fossil Energy (FE) mission. We actively maintain five technical competencies in which we conduct research and development (R&D) as a national laboratory to show best-value execution and impact from our work. Each competency complements the others, and by working together, advances technology to meet our sponsor's research needs.

Through research in ***Energy Conversion Engineering***, we develop new technologies and processes for converting fossil energy into power, fuels and chemicals, and for separating particulates and gases. We focus on specific end-use problems and how to integrate our results into energy systems.

Materials Science and Engineering research develops novel materials for extreme service environments by engineering structural and functional materials with targeted characteristics. We design, discover, synthesize, characterize, process, and test materials for proof of concept in advanced power systems.

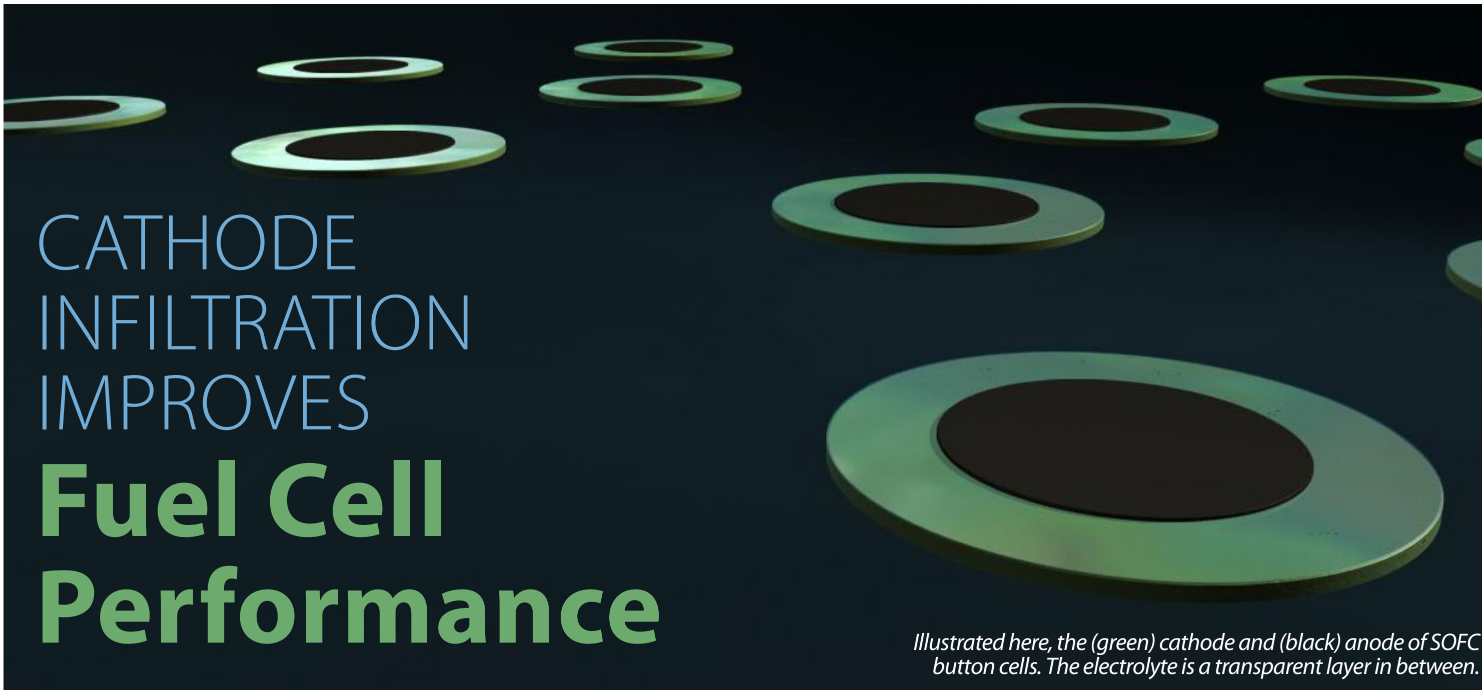
Computational Science and Engineering research addresses technical barriers to next-generation technologies via a simulation-based approach. By developing and employing models, methods, algorithms, and software tools, and integrating experimental information with models, we gain understanding beyond the reach of experiments alone.

In the ***Geological and Environmental Science*** realm, we leverage expertise in geomaterials science, fluid flow in geologic media, multi-scale assessments, geospatial data management and analyses, and strategic field monitoring. Subsurface research efforts generate knowledge and technologies needed for sustainable development and utilization of domestic energy resources.

Safe, Fiscally Responsible Research and Development is assured by crosscutting resources that provide support to our R&D functions. These resources manage the Safety Analysis and Review System, as well as design, construction, modification, operations, and decommissioning of R&D facilities.

Randall Gemmen
Associate Deputy Director of Research & Development

Cover image
3D Rendering of NETL's Multi Cell Array, which accelerated cathode infiltration development by enabling statistically significant parallel testing.



CATHODE INFILTRATION IMPROVES Fuel Cell Performance

Illustrated here, the (green) cathode and (black) anode of SOFC button cells. The electrolyte is a transparent layer in between.

Solid oxide fuel cells (SOFCs) address the environmental and climate change concerns associated with fossil fuel based electric power generation. However, reliability and affordability have traditionally impeded SOFCs from gaining broad commercial interest. SOFCs are expensive and, because they operate at high temperature, tend to degrade quickly. To better understand how to improve these factors, NETL researchers investigated how and where the chemical reactions take place within SOFCs. What they discovered is that improving cathode performance can significantly impact the overall performance and cost of a fuel cell system.

To improve cathode efficiency, NETL's Fuel Cell Team developed a special technique called infiltration to intensify the power-producing reactions inside the cell. "SOFC structure and catalytic function are closely coupled," says **Dr. Kirk Gerdes**, NETL's Fuel Cell Research Team Lead. "Infiltration gives us control over performance by allowing control over the active electrode structures." Cathode infiltration involves depositing an electrocatalyst on the cathode in the precise location needed to facilitate reactions and improve the ratio of electricity produced to fuel consumed. The team developed a nanoscale electrocatalyst to provide electrocatalytically active materials to the cathode. Nanoscale materials offer large surface areas, which means more of the electrocatalyst material can contact the cathode, increasing reactivity.

Dr. Shiwoo Lee uses NETL's sonic spray coater to apply electrocatalyst solution to a fuel cell cathode.

In the lab, the electrocatalyst is applied by hand to each individual cell. But this is not an option for mass application of cathode infiltration to SOFCs. NETL researchers realized that further innovation was needed to transfer the technology to industry, and they developed a manufacturing method for their infiltration technology.

Screen printing is the typical manufacturing process for SOFC electrodes. Liquid "paints" made from cathode materials are printed onto the cell, much like printing a design onto a t-shirt. While SOFCs produced this way are cheap and the electrodes are produced with uniform size and shape, screen printing limits control over where a fuel cell's active sites (the sites where reactions occur) will be distributed. A more precise manufacturing method was needed if cathode infiltration was to be a viable solution to improving SOFC performance and efficiency and to position this technology for the commercial market.

The team's investigations of the internal SOFC structure resulted in complete and detailed 3-D maps of active components, and they applied that

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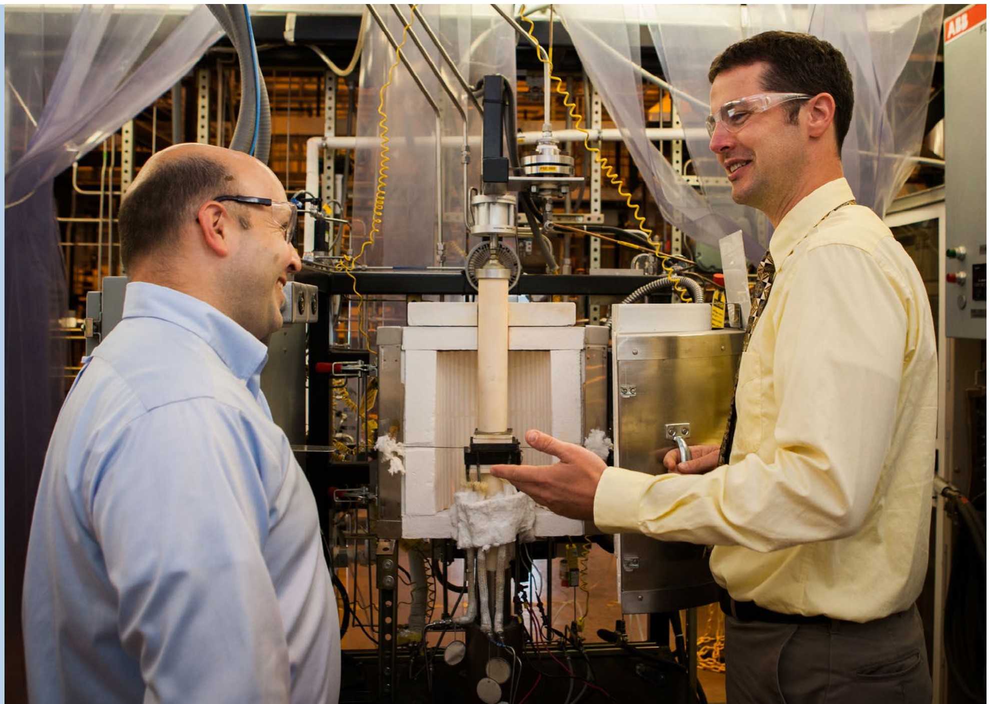
knowledge to determine exactly where the electrocatalyst should be placed for superior performance. Next, the NETL engineers designed a novel process that uses a spray coating machine (see box, below) coupled with special computer software to mass produce infiltrated SOFCs possessing a precisely controlled electrode structure. The cathode can be built layer by layer, placing active structures at exact locations for optimal functionality so that the reaction networks are constructed in a sequential way. The electrocatalyst is applied in a solution over the cathode. The team is able to cheaply and precisely control how much infiltrate is applied to achieve the desired performance, resulting in new fuel cells that cost less per kilowatt generated, are more efficient, and more durable. According to Dr. Gerdes: "The manufacturing process is critical to helping make this technology commercially competitive. We can now better engineer performance, and the advanced manufacturing process produces an optimal fuel cell."



Dr. Harry Abernathy and Dr. Kirk Gerdes investigate reactions inside a fuel cell stack.

By optimizing reactions inside the cell, cathode infiltration methodology developed by NETL's Fuel Cell Team can dramatically improve efficiency and performance of SOFC, ultimately reducing costs and launching SOFCs into the commercial market.

Contact: [Kirk Gerdes]

Sonic Spray Coater Builds Better Fuel Cells

NETL fuel cell researchers use a unique sonic spray coater to infiltrate cathodes of solid oxide fuel cells. This spray coater uses a sonic nozzle to deposit electrocatalyst solution onto the fuel cell, whereas conventional aerosol coaters use a high-pressure gas to distribute material. The sonic spray coater vibrates at a set frequency, shaking off droplets from the tip of the nozzle. The resulting low-velocity impact improves spray control and eliminates risk of damage to the fuel cell components. Researchers also control the infiltrate chemistry deposited by the sonic nozzle. As a result, the sonic spray coater gives fuel cell researchers tight control over the deposited material enabling production of a finely engineered fuel cell.

NETL's sonic spray coater deposits electrocatalyst solution onto a 300-watt SOFC.

Location, Location, Location: An Oil Spill Comparison

Image courtesy of the U.S. Coast Guard.

Dark clouds of smoke billow as oil burns during a controlled fire in the Gulf of Mexico on May 6, 2010. The Deepwater Horizon oil spill was the largest accidental marine oil spill in history.

Understanding the risks associated with offshore oil exploration and production is key to preventing oil spills that jeopardize wildlife and mankind. To determine what elements are most important to reducing the potential risks, researchers conducted a baseline study comparing the two largest single source oil spills in U.S. history: the Exxon Valdez tanker in Prince William Sound, Alaska, and the Deepwater Horizon oil rig in the Macondo prospect in the Gulf of Mexico. **Jennifer Bauer**, a Geospatial Analyst at NETL, worked on the project. "We started looking at the spills, comparing cleanup efforts to their impacts, and what we found that wasn't already discussed in the literature, was that location matters. The length and duration of environmental and social community impacts varied based on where the spill occurred."

The study, published in the *Journal of Sustainable Energy Engineering* this past September, was a collaborative effort by Bauer; **Kelly Rose**, who leads the Geology & Geospatial Team; and post-grad ORISE fellow **Jake Nelson**. "The collaboration allowed us to leverage our individual expertise and combine them to the greatest benefit," said Bauer. She explained that Nelson's geographic background assisted in understanding how the different geography of the regions affected the spills; Bauer's background in marine biology, and Rose's strong understanding of hydrocarbon extraction in deepwater environments contributed complementary perspectives to the paper's analysis and conclusions.

The team compared multiple aspects of the two spills and examined the impact of location to both the cleanup efforts and the incidents' long-term impacts. The lack of infrastructure in Prince William Sound complicated the mobilization of responders compared to cleanup efforts in the Gulf of Mexico. But beyond the people involved, differences in the ecosystem also played a role. The Gulf of Mexico is an ideal home for oil-eating bacteria that do not flourish in the colder Alaskan waters. Location can also affect the severity of impacts. "In Prince William Sound, even after cleanup, the spill greatly affected the fisheries, to the point where some almost collapsed for certain species. In the Gulf of Mexico, similar impacts to the fisheries haven't yet been observed," says Bauer.

In the end, Bauer is cautiously optimistic. "Since we know that location matters, we can begin factoring location into our analyses . . . and use this knowledge to help guide oil spill prevention efforts as well as recommend response to any future oil spill events."

Contact: Jennifer Bauer

Filling the Knowledge Gap to Accurately Predict Deepwater Hydrocarbon Behavior

Deepwater drilling is the process of oil and natural gas retrieval from underwater reserves located thousands of feet beneath the ocean's surface. Consequentially, deep reservoirs are under intense pressures and extreme temperatures that are rarely found in other environments. Although deepwater drilling efforts began in the 1990s, we still have clear knowledge gaps in our understanding of how hydrocarbons behave under such extreme conditions.

Knowledge gaps, or missing pieces in the existent body of knowledge on a subject, are pervasive in the field of deepwater hydrocarbon research. One reason for this dearth of information was the lack of laboratory equipment capable of simulating the extreme conditions of deep and ultra-deepwater environments and therefore generating data that could be used to create models of hydrocarbon behavior at those depths.

In direct response to these unknowns, NETL created the Equation of State (EOS) Research Team. The team works on the Ultra-Deepwater and Offshore Research and Development portfolio, the Department of Energy's concerted research effort to address knowledge gaps that may negatively impact the safe and efficient production of oil and gas from these reservoirs.

Though NETL scientists manage and lead the EOS Research Team, team members are drawn from multiple organizations, including both the University of Pittsburgh and Virginia Commonwealth University. Headed by **Dr. Isaac Gamwo**, the team's primary directive is to develop equations of state for hydrocarbon fluids capable of predicting the pressure, volume, and temperature behavior of a substance.

To address these issues, the EOS team have designed, constructed, tested, and operated two different experimental cells—a high-temperature, high-pressure densimeter (see image) and a high-temperature, high-pressure rolling-ball viscometer—both capable of withstanding conditions up to 500 °F and 40,000 psi. These cells are used to measure the density and viscosity of pure hydrocarbon components and crude oil at conditions encountered several miles beneath the sea floor.

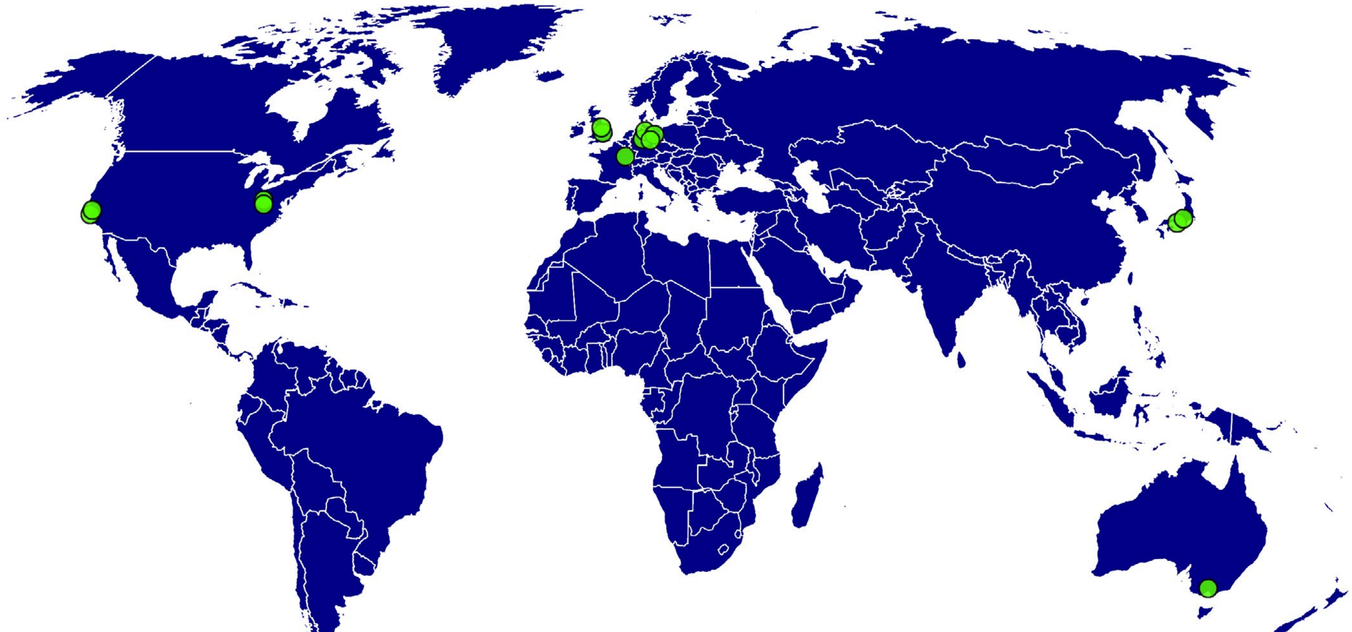
Currently, the cells developed by the EOS Research Team are unmatched by any other research group in the world. The cells have made it possible for the research team to collect the fundamental data needed to understand fluid behavior at deepwater reservoir conditions. Better understanding fluid behavior enables development of innovative technologies to further expand the acquisition of domestic natural gas and oil from ultra-deep reservoirs. The findings produced by the EOS Team are also benefitting thermodynamic research in Spain, Greece, France, Australia, and the UK.

Dr. Gamwo views the progress of his group as success, not just for NETL, but for the international energy industry. "Filling the density and viscosity database for hydrocarbons at extreme conditions has placed NETL in the forefront of research, but the results are providing benefits on a global scale. I'm privileged to be a part of this research effort."

Contact: Isaac Gamwo

NETL's high-temperature, high-pressure densimeter.

Inter-laboratory Comparison Studies Lead to Establishment of Best Practices



Organizations around the world (indicated by green circles) participated in an international, multi-laboratory study focused on comparing results of geochemical reactions in a CO_2 storage reservoir.

Inter-laboratory comparison studies are commonly used to evaluate reproducibility and accuracy of results obtained using different experimental approaches. Such studies provide direct assessment of variations across different laboratories and allow the research community to identify laboratories producing dissimilar results. Differences in the results are studied with the goal of understanding what factors contribute to the variation in data, identifying problems, and crafting methods to mitigate the cause of the variance. This type of study is an important part of a laboratory's quality assurance program and can serve to verify a lab's analytical approach. NETL has a history of participating in large research projects that use data collected from multiple laboratories. Obtaining a better understanding of inter-laboratory variation is important to the integrity of the research and for establishing best practices.

NETL is currently engaged in a large multi-laboratory investigation of the effect of carbon dioxide (CO_2) injection in deep saline formations systems. Understanding the effects of injected CO_2 on the chemical and physical properties of a subsurface system is important to establishing long-term safety and permanent storage of CO_2. Determining the in situ effects of carbon injection at real reservoir sites is a difficult and expensive undertaking and serves as the impetus for developing laboratory-based model systems. Developing relevant experimental models that mimic natural reservoir systems is an active area of research worldwide with different analytical approaches being evaluated. Designing laboratory systems that control for key variables including temperature, pressure, salinity, and mineral composition can provide operating systems capable of yielding relevant geochemical and geophysical data. However, ensuring consistency of measurements across multiple labs is important to ensure proper interpretation and extrapolation of experimental results.

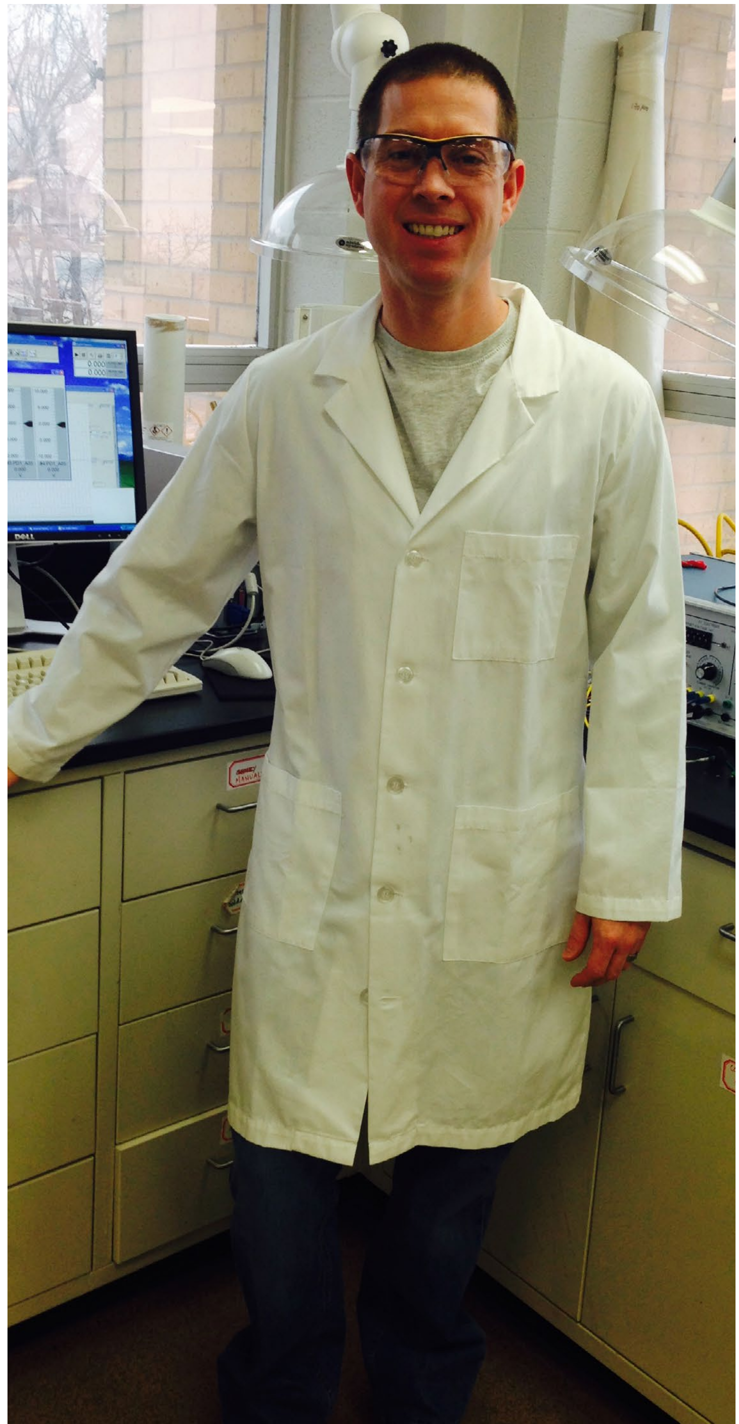
Dr. Angela Goodman, NETL's technical portfolio lead for Carbon Storage, noted, "In addition to strengthening international collaboration and data sharing, inter-laboratory comparison studies provide an estimate as to how much different experimental approaches vary in their results. The ultimate result of these studies will lead to development of more robust and predictable analytical methods at NETL as well as at other laboratories across the globe."

NETL researchers recently participated in an inter-laboratory geochemical comparison study involving 14 laboratories from six countries. Organized and led by the Federal Institute for Geosciences and Natural Resources (Hanover, Germany) and the U.S. Geological Survey (Menlo Park, CA), the study was designed to compare different experimental approaches for evaluating the effects of CO_2 on brine-mineral geochemical characteristics. Overall, the results recorded across the labs show similar trends indicating a level of consistency among individual laboratory approaches. The team is planning a follow-up comparison study to evaluate additional variables in an attempt to establish best practices for the evaluation CO_2-brine-mineral interaction. As Dr. Goodman explains, "Development of predictive tools for CO_2-brine-mineral interaction will aid in reducing uncertainty associated with CO_2 storage, ensuring safe and permanent storage of CO_2."

Contact: Angela Goodman

Intern's Research Improves Manufacturing and Commercialization of Solid Oxide Fuel Cells

When **Regis Dowd**, a research associate from the University of Kansas, first arrived at NETL, he was curious about how research performed at the laboratory actually resulted in measurable benefits to Americans. Now, after 8 months working with researchers in the Fuel Cells Laboratory, Regis not only understands the value of NETL's energy research, he has actively contributed to its transfer from laboratory to industry. Regis's work on improving the manufacturing and commercialization of solid oxide fuel cells (SOFCs) is helping to position the nation to produce energy more efficiently and with lower energy costs.


Regis Dowd, a doctoral student in chemical engineering at University of Kansas.

As part of his internship with the Fuel Cell Research Team, Regis developed a method to improve the performance of SOFCs while minimizing manufacturing costs. He focused on developing a one-step infiltration process, which involves delivering specific amounts of nanocatalyst to the cathode of a SOFC. By manipulating key variables in the process, Regis endeavored to create a cost-effective manufacturing method applicable to commercial SOFCs. And after devoting months of careful work, Regis succeeded in simplifying the process to infiltrate SOFCs.

Industry is now more likely to adopt this infiltration process because it addresses the most difficult hurdle to commercializing new SOFC technologies—the manufacturing cost. **Dr. Kirk Gerdes**, a fuel cell researcher at NETL and Regis's co-mentor, says of Regis's achievement, "The process Regis created with our team pushes our laboratory-developed technology closer to the marketplace by increasing throughput while adding less than a half percent to cell costs." Co-mentor **Dr. Shiwoo Lee** concurs, and notes "Regis's dedicated effort accelerated the rate at which we obtained a viable engineering solution."

Regis feels grateful to have been a part of this process and credits the preeminent fuel cell researchers at NETL for providing the base of knowledge that he used to bridge the gap into potential commercialization. "My internship was a great experience. I was able to directly observe how research at a national laboratory can go from inception to commercialization. I hope that our discoveries will lead to greater use of SOFCs, which will benefit the nation," Regis said about his time at NETL.

Regis and the fuel cell team are currently working on filing a patent for the one-step infiltration process and publishing their research.

Take a virtual tour of SOFC laboratory here.

Contact: Kirk Gerdes

NETL's In-House Research Program: Fuel Cells

Solid oxide fuel cells (SOFCs) have positive and negative aspects—literally and figuratively—with each SOFC having a positively charged electrode (called a cathode) and a negatively charged electrode (anode). Fuel and oxygen molecules that pass between the electrodes interact with catalysts, an electrolyte, and each other to generate electricity, water, and carbon dioxide (when using a carbon-containing fuel). Compared to conventional power production technologies, SOFCs generate electricity at much higher efficiencies, resulting in significantly reduced carbon dioxide emissions and lower fuel consumption. The disadvantage is that technologies that make SOFCs practical—on a large scale—are expensive. The technologies must also be able to withstand temperatures of up to 1,000 degrees Celsius, hot enough to melt glass or harden pottery. NETL researchers are working with the Solid State Energy Conversion Alliance (SECA) to pursue more affordable and durable SOFC technologies. They are investigating how SOFC components degrade over time and inventing stronger, better-performing electrodes. Their work comprises the following tasks:

- Analyze how different conditions (such as humidity and overpotential) can degrade an electrode through the use of computational and physical models and advanced, high-resolution microscopy and spectroscopy.
- Collaborate with SECA members to increase the accuracy of SOFC models and then test them on NETL's supercomputer.
- Create and improve SOFC models by developing computational "bridges" that link atomic-scale phenomena inside an SOFC to its measurable properties, and create the SOFC Hurricane Model, which predicts how an SOFC stack operates over its service life.
- Conduct laboratory testing to develop electrodes that increase fuel cell power output and meet the needs of SECA industrial partners.

For more information about this research, contact Kirk Gerdes.

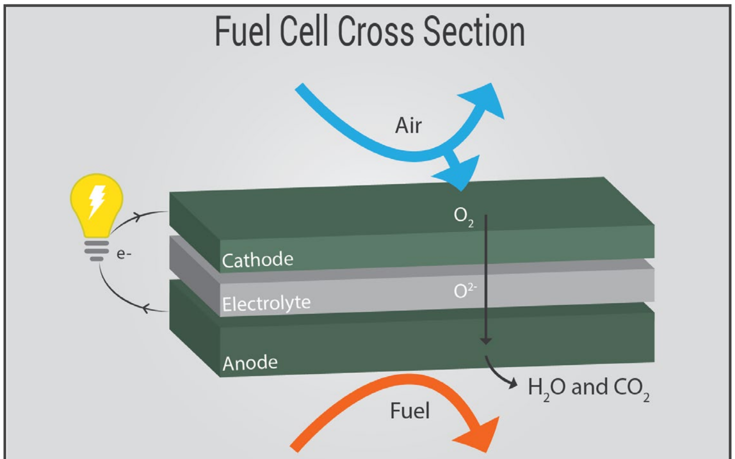
FUNDAMENTAL FUN

Solid Oxide Fuel Cell Basics

Fuel cells are electrochemical devices that convert the chemical energy of a fuel (such as methane) and oxidant (such as air) directly into electrical energy. Fuel cells consist of three layers: an anode, an electrolyte, and a cathode. But a fuel cell is not a battery. Batteries store energy and must be recharged when they run out of juice. Fuel cells convert chemical energy to electricity and will continue to operate as long as fuel is supplied.

In a solid oxide fuel cell (SOFC), air enters the cathode and fuel enters the anode. The electrolyte, which in a SOFC is a solid ceramic material, conducts oxygen ions from the cathode, which meet—and react electrochemically—with fuel from the anode side. The oxygen ions combine with the fuel to produce an electrical current, water, and carbon dioxide (CO_2).

What makes SOFCs a good fit for fossil energy applications is that they can use both hydrogen and carbon monoxide, which are produced during coal gasification, in the electrochemical reaction. Because there is no combusting of fuel, the fuel cell generates virtually no harmful emissions. This results in power production that is almost entirely absent of nitrogen oxide, sulfur dioxide, or particulate matter. Plus, SOFCs are ideal for carbon capture because the fuel and air streams are kept separate resulting in a pure stream of CO_2 and water, facilitating the capture of carbon without substantial additional gas separation costs.



In a solid oxide fuel cell, air enters the cathode, passes through the electrolyte, and reacts with fuel from the anode side to produce electricity.

A special type of solid oxide cell called an electrolyzer can produce hydrogen from water. These cells run in a mode known as "regenerative," because they add energy to water to regenerate the molecule's original elements, oxygen and hydrogen. Water at the cathode side undergoes electrolysis to form hydrogen and oxide ions. The oxide ions are transported through the electrolyte to the anode where they form molecular oxygen. The hydrogen produced can then be used for many applications, including as a fuel for SOFCs. For example, SOFCs could be used to run auxiliary power units on spacecraft and unmanned undersea vehicles that cannot be easily refueled. In this case, the devices could be switched to regenerative mode when power demand is low and the hydrogen produced then used as fuel to power the SOFCs.

APPLAUSE

Patent Issued

Visible Light Photoreduction of CO_2 Using Heterostructured Catalysts, **Robert L. Thompson** (Parsons); **Congjun Wang** (Parsons); **Christopher Matranga** (DOE/NETL); [8,986,511](), issued March 24, 2015.

Licenses for NETL Intellectual Property

KW Associates, LLC, license for U.S. Patent 8,111,059 "Arc Position Sensor" (also known as Electric Current Locator), issued on March 3, 2015.

Pyrochem Catalyst Company, license for U.S. Patent Application No 14/296,643, "Method for continuous synthesis of metal oxide powders," issued on March 25, 2015.

Kudos!

Dr. Stephen E. Zitney, an Engineer at NETL, was recently elected by the AIChE Board of Directors as a Fellow of the American Institute of Chemical Engineers. This honor affirms the high esteem with which Dr. Zitney's colleagues and peers view his distinctive professional achievements and accomplishments. He will receive his Fellows pin and plaque at the Fellows Breakfast at the AIChE's 2015 Spring Meeting on April 28th.

Highly Cited Paper

The review paper "Advances in CO_2 capture technology: A patent review" by Dr. Bingyun Li (WVU); **Dr. Yuhua Duan**, **Dr. David Luebke**, and **Dr. Bryan Morreale** (NETL), received Applied Energy's Highly Cited Award in March 2015. The paper has been cited more than 100 times since its publication in 2013. Congratulations to all of the authors!

ORD: Science & Engineering To Power Our Future

EXTRA! EXTRA!

NETL's Foamed Cement R&D was the cover story in January's Journal of Petroleum Technology, the flagship magazine of the Society of Petroleum Engineers.

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