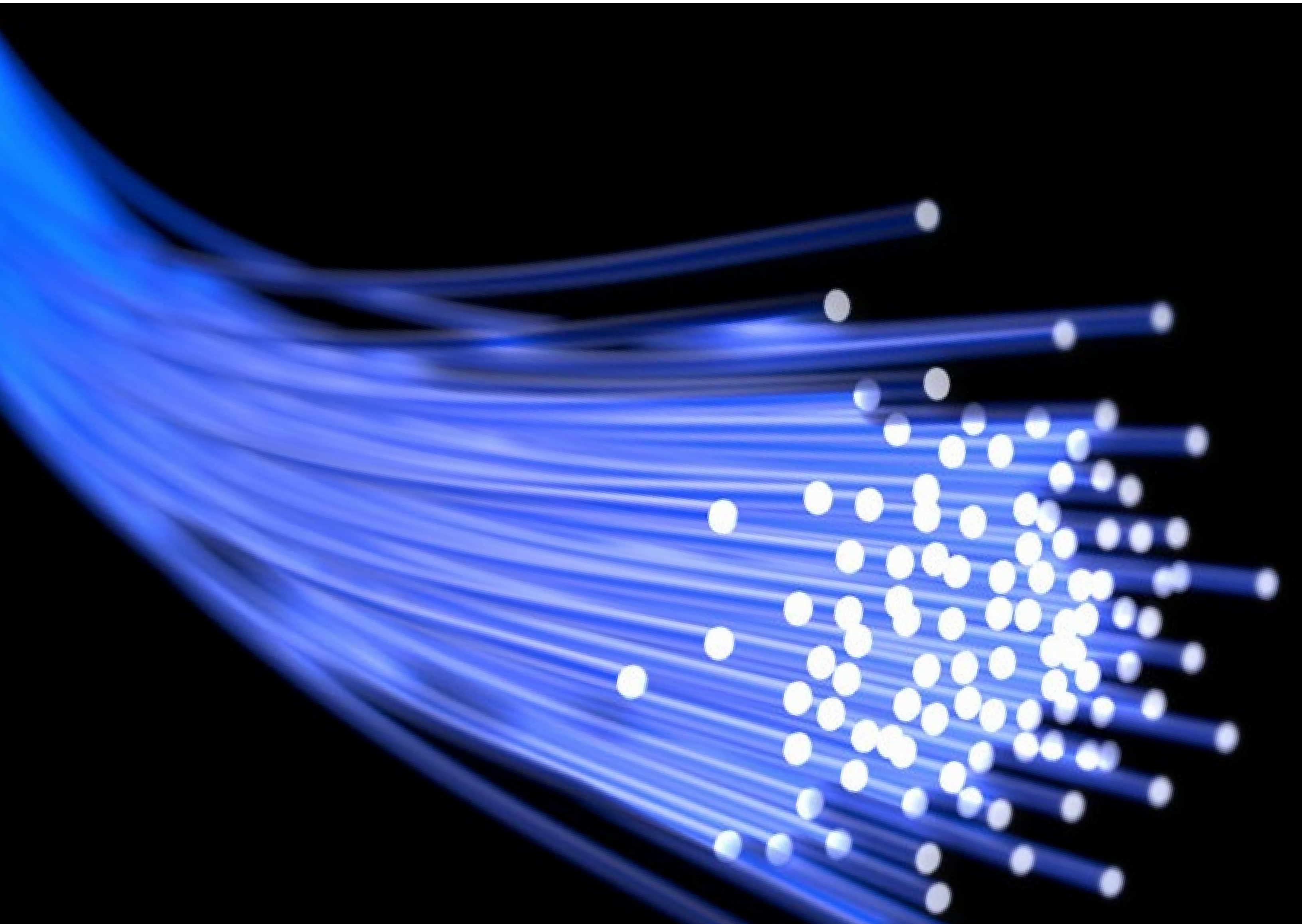
From NETL's Office of Research & Development

# Research news

May 2015, Issue 8



FOCUS STORY:

## Going to New Extremes—Application of Advanced Sensors for Subsurface Monitoring

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NATIONAL ENERGY TECHNOLOGY LABORATORY

U.S. DEPARTMENT OF ENERGY

Research news

May 2015, Issue 8

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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.

# CLEARING THE HURDLES:
# NETL's Energy Data eXchange

Communication is the foundation of any good relationship, from the romantic to the scientific, but surmounting the barriers that surround establishing fruitful research partnerships can be daunting. Data sets are often too large to be easily transferred between organizations and secure workspaces are not always accessible. NETL's Energy Data eXchange, or EDX, is designed to help scientists foster the communication that undergirds successful, collaborative research.

Borrowing from the concepts that made social networking tools a success, EDX is, in essence, a knowledge-sharing tool, designed to house and connect users to energy-related datasets, key tools to support data analysis and evaluation, and to host secure team collaborative workspaces that can streamline research partnerships.

"EDX isn't simple to condense into one function, because it was designed to meet multiple needs simultaneously," said **Kelly Rose**, research geologist and EDX coordinator. "At its heart, EDX is a tool. It's online, it has a web interface – but behind the scenes? It's a tool, developed by researchers for researcher-related needs and to facilitate discoverability, accessibility, and utility of the data, tools, and functions multi-organizational teams need every day to address energy related technical challenges."

There are approximately 500 users in the EDX community, comprising internal users and external collaborators in approximately equal numbers. The number of EDX users has grown considerably since its introduction and continues to expand. EDX currently stores about 7,000 energy-related data resources, and provides access to over 200,000 data resources through its federated search functionality. The federated search function allows users to look for relevant datasets that are hosted by other parties.

Data loss is a serious problem that plagues the research community. The primary datasets that underpin most peer-reviewed research publications are lost over time, becoming essentially inaccessible as little as five years after a publication's release. EDX is a simple way to counteract this trend, by preserving datasets and keeping them accessible even as time passes.

*...Continued on page 3*

**Cover image**

NETL's Advanced Sensors Development Laboratory is developing new sensor technology for applications in subsurface monitoring.

A growing number of NETL research portfolios are using and being transformed by EDX. For example, the Offshore Energy Resources team uses EDX as it develops a scientific base for reducing and quantifying potential risks associated with exploration and production of oil and gas in offshore environments. The National Risk Assessment Partnership—a multi-agency initiative—also uses EDX in its efforts to develop a defensible, science-based quantitative methodology for determining risk profiles at $CO_2$ storage sites.

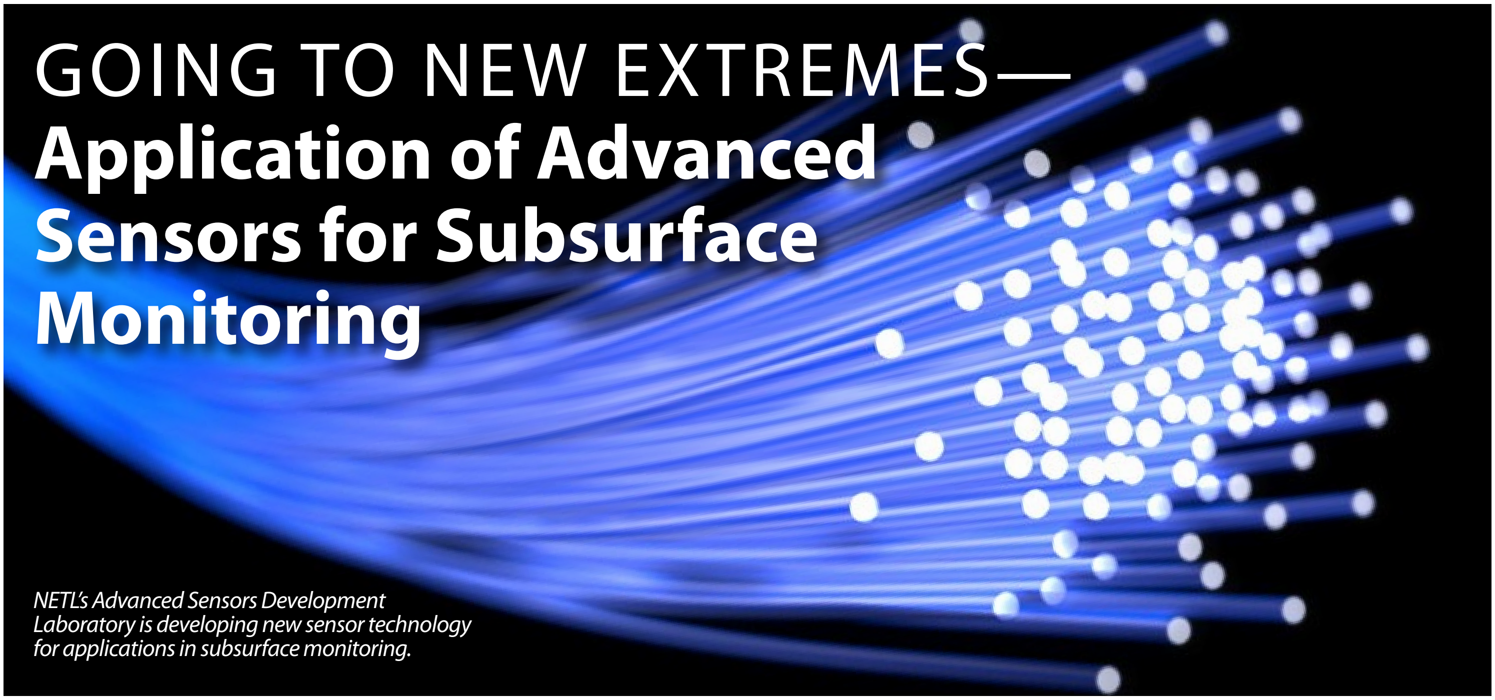

*This infographic helps illustrate the many uses of EDX.*

But EDX is not just for researchers to communicate and collaborate with each other. The platform is also a key tool in NETL's efforts to comply with the DOE Public Access Plan. The Public Access Plan was developed in response to a memorandum from the Director of the White House Office of Science and Technology Policy, Dr. John Holdren, "Increasing Access to the Results of Federally Funded Scientific Research." The memo directed federal agencies with more than $100 million in annual conduct of research and development to develop plans for increasing public access to peer-reviewed scientific publications and digital data resulting from federally funded research investments.

**Lilas Soukup**, a public affairs specialist, is leading NETL in understanding and complying with the requirements of the Public Access Plan as NETL's science and technical information manager. She thinks EDX has great potential for public knowledge transfer. "EDX is a valuable method that NETL is utilizing to adhere to the requirements laid out in the DOE Public Access Plan. EDX includes a vast compilation of scientific research information in a user-friendly format, which assists in making appropriate, unclassified data publicly accessible." EDX provides a secure platform for research collaboration while also serving as a functional tool that enhances knowledge transfer. As its user base steadily grows, EDX will continue to evolve to meet the changing needs of its community. To discover how this tool might support your technical energy data resource needs and efforts, visit EDX, and perhaps, even share your own thoughts on how to keep EDX contributing to energy R&D's present and future.

Contact: Kelly Rose

# GOING TO NEW EXTREMES—Application of Advanced Sensors for Subsurface Monitoring



*NETL's Advanced Sensors Development Laboratory is developing new sensor technology for applications in subsurface monitoring.*

At NETL, one of the Functional Materials Development Division's traditional focuses is developing sensors capable of operating in the high temperatures and harsh environments associated with fossil fuel-based power generators. A new multidisciplinary and cross-organizational effort, undertaken in NETL's Advanced Sensors Development Laboratory, has taken aim at expanding the application of advanced fiber optic sensor technology into new areas, such as carbon storage and unconventional, deep, and ultra-deepwater oil and gas resource recovery.

The laboratory serves as a bridge between basic and applied research in an effort to accelerate sensor development and deployment. The centralized facility leverages a team of materials scientists, chemists, and engineers with unique laboratory capabilities to fabricate sensors for use in the most aggressive environments. Among the lab's new capabilities are automated high pressure and high temperature reactors, which replicate subsurface environments. Lead Research Engineer **Thomas Brown** explained that "These reactors will aid in developing new sensor capabilities by providing real-time information relevant to monitoring drilling processes, well-bore integrity, and carbon dioxide ($CO_2$) migration during geological storage."

The team's initial emphasis has been placed on real-time pH monitoring. According to Engineer **Dr. Paul Ohodnicki**, "pH is the single most important parameter in determining a range of geochemical reactions in subsurface environments." While a variety of options is available for pH measurement under biological or ambient conditions, no reliable pH sensing techniques are available for wellbore and $CO_2$ storage applications.

Exploiting the unique advantages of a combination of material chemistry and fiber optics, Chief Material Scientist **Dr. Congjun Wang** and his colleagues developed and demonstrated several new fiber optic-based pH sensing approaches that will allow for embedded, real-time, remote pH sensing capabilities in extreme subsurface environments.

Monitoring the pH of wellbores and $CO_2$ storage sites provides useful information on the geochemical conditions in the reservoir. According to **Dr. Barbara Kutchko**, a physical scientist in NETL's Materials Characterization Division and a wellbore cement integrity expert, "An acidic reservoir environment may lead to cement alteration and wellbore corrosion, which can lead to operational failure. The ability of the well operators to monitor and adjust wellbore chemistry conditions will lead to improved oil and gas recovery while ensuring the functional integrity of the well."

When applied to monitoring $CO_2$ storage sites, Geochemist **Dr. Alexandra Hakala** of NETL's Engineered Natural Systems Division noted, "$CO_2$ can acidify storage formation waters, inducing mineral breakdown and precipitation reactions, which ultimately affects long-term $CO_2$ storage permanence." **Dr. Christina Lopano**, geochemist, described other potential effects $CO_2$ may have on water. "If $CO_2$ migrates from the storage formation to shallow ground waters, changes in pH can affect mineral solubility and trace metal mobility, which can affect water quality. The ability to monitor the pH will allow us to better determine impacts associated with subsurface $CO_2$ storage." Physical Scientist **Dr. Angela Goodman** added, "Advanced fiber optic sensor technology will be beneficial for developing tools and protocols for protection of groundwater resources by identifying potential $CO_2$ or brine intrusion in aquifers. Monitoring of underground sources of drinking water is crucial to the successful implementation of geologic carbon storage."

NETL has developed a portfolio of advanced optical sensor materials that address process monitoring in harsh environments. These technologies are available for licensing and/or further cooperative development through NETL's Technology Transfer. You can learn more about the team's work in developing fiber optic sensors for pH monitoring by reviewing their recently published article in *Nanoscale*.

Contact: Paul Ohodnicki

# Researchers Follow an Atomic Map to Success

NETL has recently added a valuable new capability of analyzing single-crystals to its materials characterization toolset that has already led to discoveries in the fields of $CO_2$ reuse and high-temperature sensing. The Materials Characterization Division (MCD) of NETL previously housed an x-ray diffraction instrument, but when a software component was recently upgraded, the machine gained considerable new features including the ability to analyze single-crystal as well as polycrystalline materials. After collaborating with the Molecular Science Division (MSD), which contributed its expertise in single-crystal growth and diffraction measurements, the team set to work on analyzing materials with a higher degree of accuracy.


*Jonathan Lekse and Christina Lopano stand next to the x-ray diffraction instrument.*

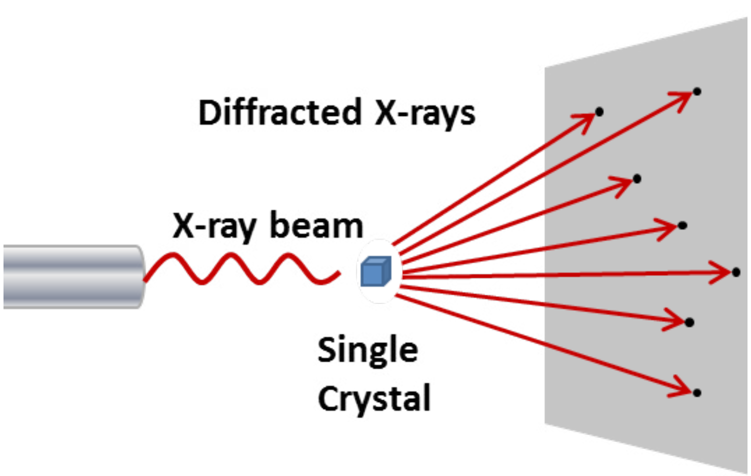
In x-ray diffraction analysis, researchers use crystalline samples of the material of interest, because crystals have a regular, ordered structure, which is crucial for acquiring meaningful data. X-rays are fired into the sample, and as the x-rays diffract (scatter a beam of light), they hit an image plate detector, leaving spots in the case of single crystal samples and ripples with polycrystalline samples. These marks are like a photograph of space that researchers can interpret with software to reveal the locations and structures of the atoms within the crystalized material in three dimensions.

The 3-D map of atomic locations that x-ray diffraction provides can be used to predict a material's mechanical, thermodynamic, optical, and chemical properties. This information is integrated into computational models that will determine the suitability of the material for a given application, saving time and money by targeting experimental materials that exhibit desired characteristics.

With this atomic roadmap, NETL researchers like **Jonathan Lekse** have worked with computational modelers to determine things like which catalysts may yield the best results for $CO_2$ reuse technology and what sensor materials will perform well in high-temperature applications. "These diffraction measurements allow researchers like myself to make valuable advancements in material characterization," said Lekse.

The benefits of these new capabilities extend beyond just MCD and MSD. "These new capabilities have been used for a lot of new areas that have benefited researchers throughout NETL," said Research Physical Scientist **Dr. Christina Lopano**.

Contact: Christina Lopano and Jonathan Lekse




*X-rays are diffracted from a single crystal, and the spots they create on the imaging plate are used to determine the atomic structure of the crystalline material.*

*The Rigaku D/Max Rapid II x-ray diffraction instrument can now be used to analyze single-crystal samples thanks to a recent software upgrade.*

# Surfactant Helps to Breathe New Life into Oil Wells

When oil companies first begin producing from a reservoir, the oil flows due to a combination of natural underground pressures and pumping at the surface. As oil is removed, pressures decrease until the oil no longer flows easily. Much more oil may remain—up to 90 percent— but retrieving what is left is more difficult and costly. During the next phases, oil producers recreate the pressure underground that once displaced the oil by injecting a gas or liquid into the reservoir. In the case of carbon dioxide enhanced oil recovery ($CO_2$-EOR), it is $CO_2$ that is injected. $CO_2$ is capable of recovering oil that other pressurizing fluids, such as water or nitrogen, would not be able to displace.

$CO_2$-EOR has been successfully used for decades to extend the lives of oil fields, but the technique does present challenges. Some layers of an oil reservoir may be more permeable (allowing liquids or gases to pass through) than others. When this is the case, the injected $CO_2$ will preferentially flow into these high-permeability "thief zones," which have been depleted of oil, rather than into the oil-rich layers. This problem is known as poor conformance.

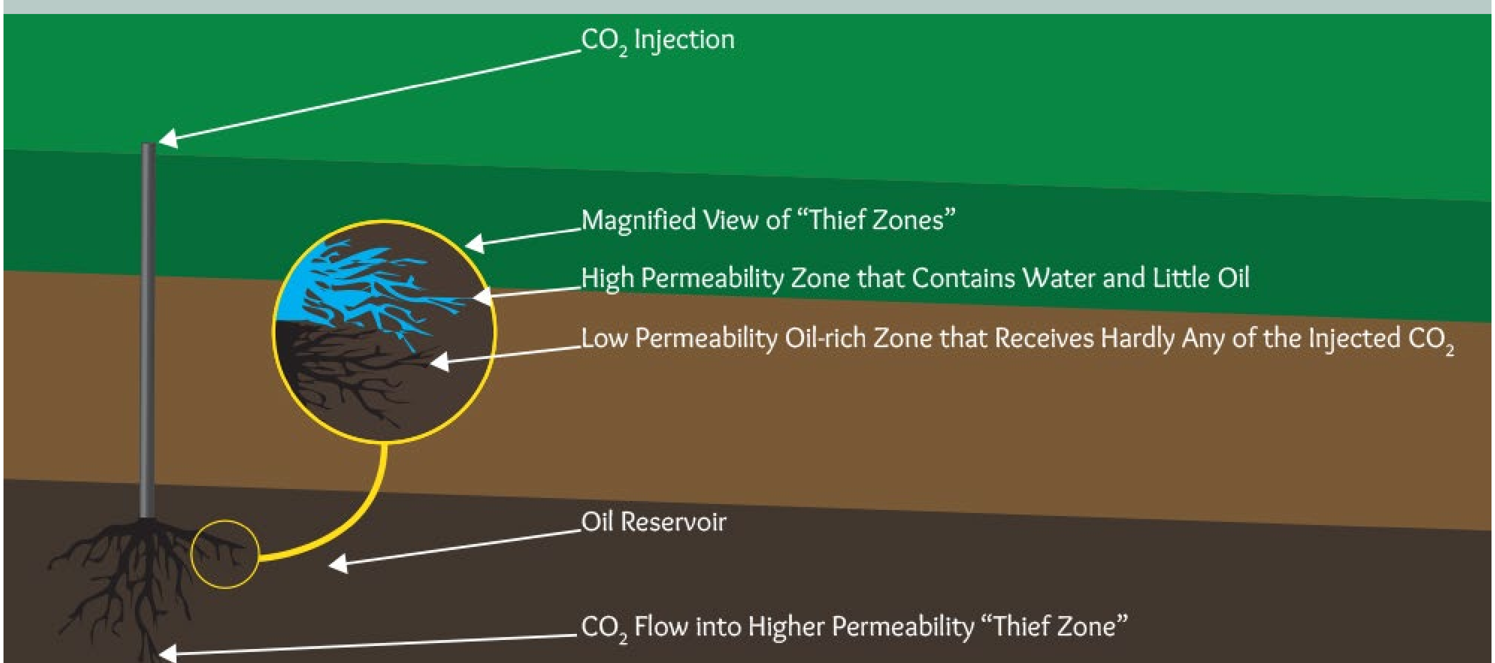
Researchers at NETL have shown that poor conformance can be reduced by dissolving a commercial surfactant (lowers surface tension) in brine (produced salty water) that mixes in the rock pores with the $CO_2$ to form foam. Surfactant stabilizes the foam by reducing the surface tension of the brine. This thick foam clogs the "thief zones" so $CO_2$ injected afterward will flow to the oil-rich, low-permeability zones, resulting in increased oil production with less $CO_2$.

To know how these foams will perform in the reservoir, researchers test core samples from the field in the Computer Tomography (CT) scanner. In the scanner, the cores are held under the same temperature and pressure observed underground, and brine containing a small percentage of surfactant is injected. They have observed distinct plug-like flow in the CT scans due to the formation of the foam. In other tests, introduction of the surfactant-stabilized foam resulted in a significant drop in pressure across the core—further indication that the foam had plugged the "thief zone." The information collected in these two tests predicted the field success of the brine-soluble surfactant.

Field tests of the technique are currently underway, and results are promising. "So far, we are seeing results in the field that closely match up with what we observed in the lab—that a commercial surfactant can be used to create foam that will improve EOR efforts," said Yee Soong, chemical engineer and principal investigator on the project.

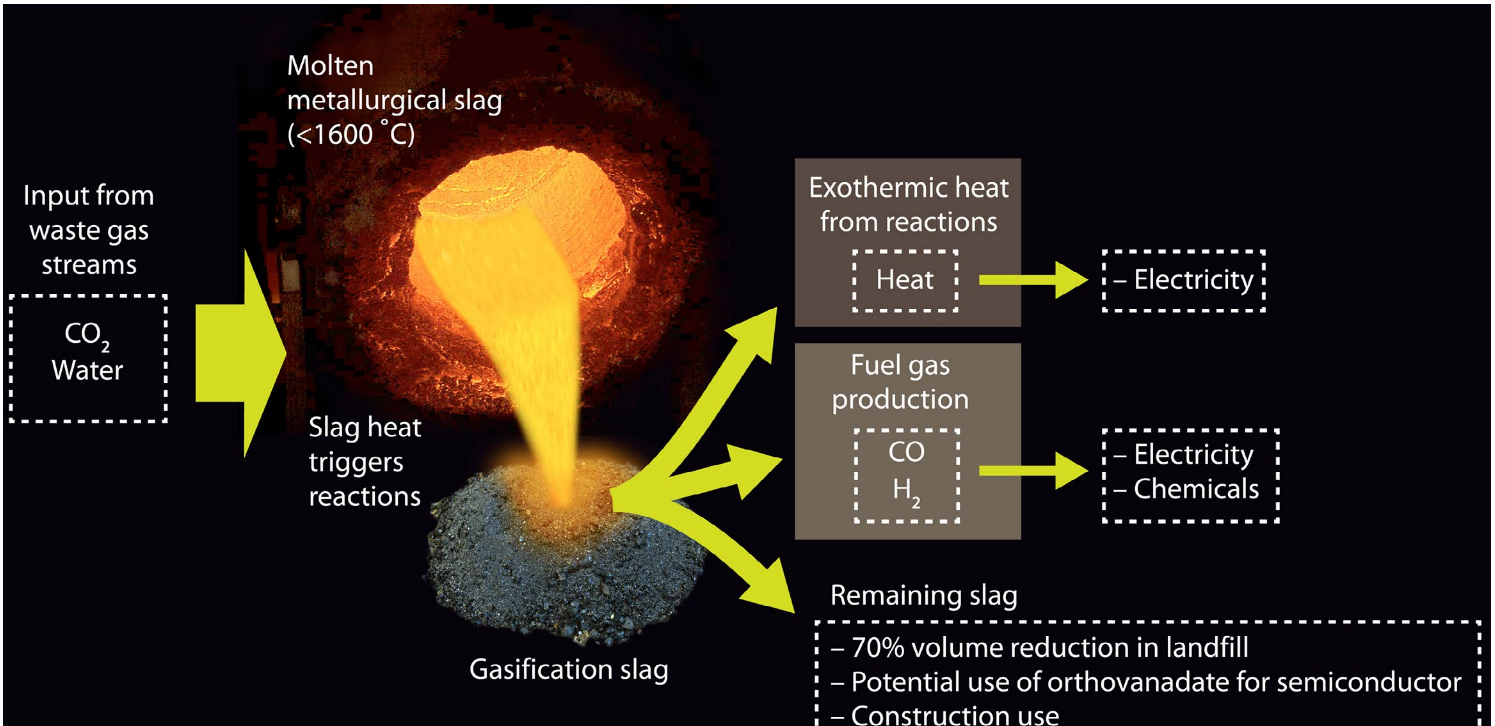
Contact: Yee Soong

*A gauge fitted on a $CO_2$ injection pipe measures pressure during an enhanced oil recovery effort.*




*Poor conformance is shown in a layered oil reservoir prior to the generation of $CO_2$ foams in the pores of the thief zone. In the magnified area, $CO_2$ entering the thief zone is shown in blue, while no $CO_2$ is seen in the oil-rich zone.*

# Making Energy from Waste While Cutting $CO_2$ Emissions




*NETL has investigated the use of waste slags for $CO_2$ reduction and fuel gas production.*

Slag—waste from power plants and steel factories—was once thought worthy of little more than dumping in landfills worldwide. Now, as a result of technology developed by two NETL researchers, it can be used as a new source of energy and help reduce carbon dioxide ($CO_2$) emissions. Different types of slags are produced as by-products from different industrial processes. For example, one type of slag waste that is produced in steel processing is high in calcium oxide from mineral impurities and fluxing agents. Meanwhile, gasification that uses petcoke carbon feedstock results in slag that contains high levels of vanadium oxide.

**Jinichiro Nakano** and **James Bennett** determined that if those two types of slag are mixed together in specific proportions upon discharge at molten temperatures in an atmosphere of $CO_2$, specific chemical reactions occur with positive implications for generating syngas (fuel), producing energy, and reducing $CO_2$ emissions.

"The chemical reaction that results from mixing the two molten slags can produce enough thermal energy for a steam turbine to generate electricity," Nakano said. "That is a more favorable use of these slags than dumping them in landfills, not to mention there is a 70 percent volume reduction after reaction."

An additional benefit to the process is that the chemical reaction converts $CO_2$, widely identified as a greenhouse gas, and $H_2O$ vapor into carbon monoxide and hydrogen. These products have value in several industries. For example, carbon monoxide and hydrogen can be used as fuel in power plants to generate electricity or as a raw material for producing chemicals like plastics or synthetic petroleum.

"Reducing $CO_2$ emissions was one of the main objectives of the research," Bennett said. The work could have global implications. Power stations and steelmaking plants are two of the largest $CO_2$ generators in the world.

A provisional patent for the technology was filed in October 2014 that addresses the broad industrial applications for the approach. Nakano and Bennett authored an article on the technology that appeared in the *International Journal of Hydrogen Energy*.

Contacts: Jinichiro Nakano and James Bennett

# Geologist Inspires the Next Generation of Scientists—Brick by Brick


As a child, **Dr. Circe Verba** used LEGO™ bricks as a foundational tool for being innovative and developing critical thinking skills. Today, she's coupling her enthusiasm for her LEGO projects with her passion for her work as a geologist and has developed a *Research Geology* LEGO set, highlighting laboratory and field work. She also developed a video about her project.

Verba was inspired after purchasing other sets offered through the LEGO Ideas campaign (e.g. Research Institute)—an opportunity for anyone to design and submit a set for consideration for production. "I wanted to entice others, particularly women, to consider a math and sciences career path," Verba said. Although recent larger efforts have been made to encourage women to enter scientific fields, those professions are still largely male-dominated. "It is important for children to see men and women working together for scientific discovery and innovation," she continued, so her set features both a female and a male mini-figure.

*Dr. Circe Verba designed her Research Geology LEGO set to include a lab much like the one she works in at NETL.*

Verba's middle school Earth Sciences class triggered her interest in science careers and led her to major in Earth Sciences at Oregon State University. After an internship at the SETI Institute, Verba pursued a master's degree at Northern Arizona University concentrating on planetary geology. Concurrent with her graduate studies, she worked at the U.S. Geological Survey's Astrogeology Branch under the NASA-funded HiRISE (High-Resolution Imaging Science Experiment) program: a camera aboard the Mars Reconnaissance Orbiter that circles Mars.

Verba's background proved useful during her ORISE internship at NETL when she used a scanning electron microscope to analyze cement-based materials. While at NETL, she obtained her Ph.D. in geochemistry in 2013 from University of Oregon.

Today, Dr. Verba is a research geologist focusing on well integrity in $CO_2$ storage and unconventional systems. Her current projects include the biogeochemical influence of microbes on sealing compromised well cement, porosity of oil-gas shale, and integration of rare earth elements and metals into cement. She also mentors ORISE and Mickey Leland interns at NETL. To bring attention to what geologists can do, Verba presents at local science-oriented events.

Already, several news sources have highlighted Verba's LEGO set, including The Oregonian, Oregon Public Broadcasting, The Albany Democrat-Herald, and Lifehacker. Verba hopes to achieve the required 10,000 votes for LEGO to consider production and distribution. To vote for Dr. Verba's *Research Geology* set, visit the page, and click on the blue "support" button on the right, which requires a free user LEGO ID account.

Contact: Circe Verba

# Navigating EDX:

## Chad Rowan's Role in the Energy Data eXchange

EDX Operations Manager Chad Rowan specializes in helping people find their way. Chad began his journey in geography, and now relies on the skills he developed as a geographic information system (GIS) expert to teach EDX users how to navigate NETL's premier data management system.

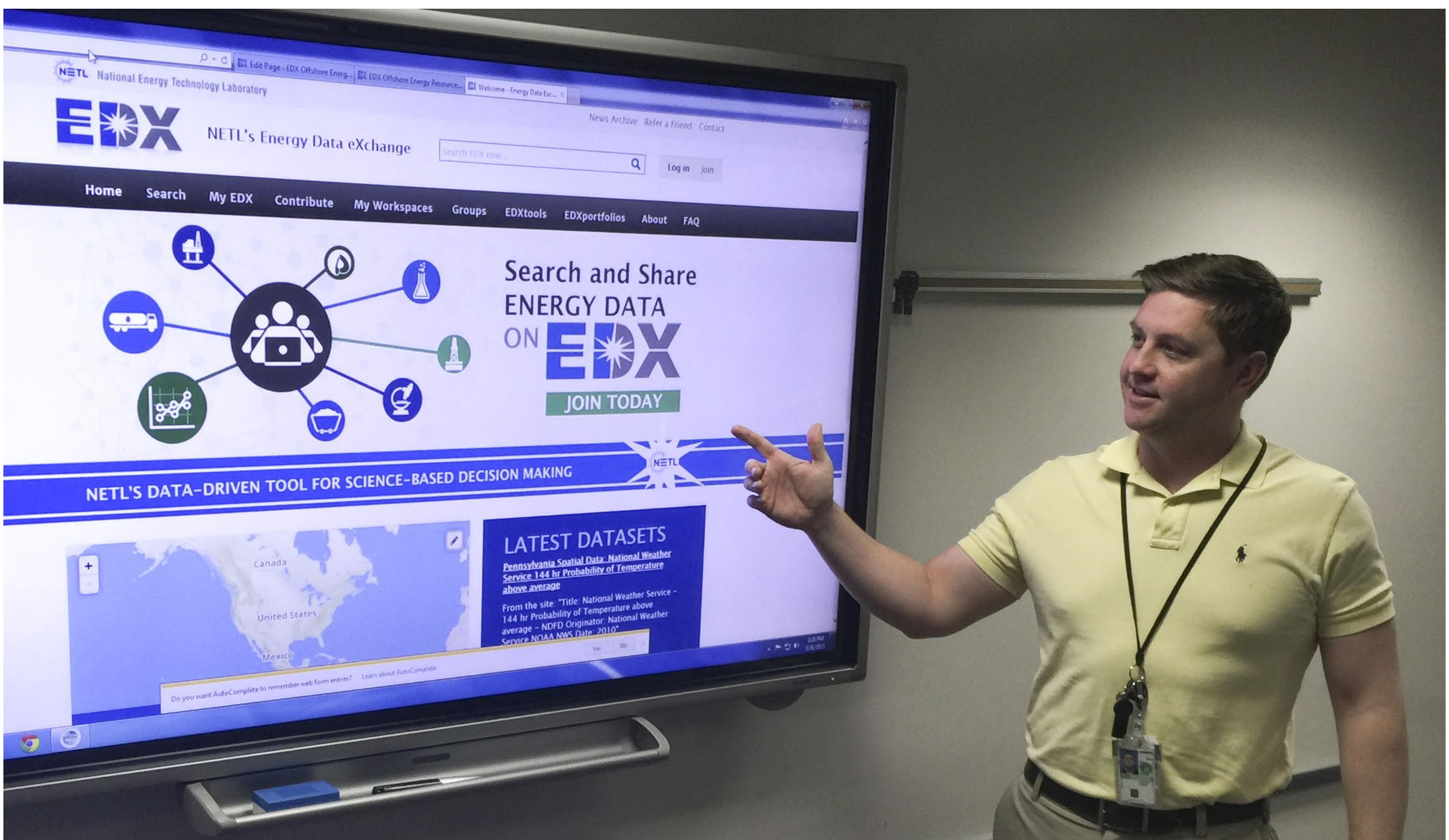
In 2011, Chad joined NETL to organize data and "brainstorm for the product that became EDX." He joined the EDX project at its inception and has been a leader in its development ever since. His specialized background in GIS and geospatial analysis—fields that gave him a thorough grounding in data management, storing, and analysis—has been a strong asset for EDX.

Today, Chad is helping others discover and navigate EDX. His responsibilities encompass creating new user accounts and giving demonstrations of the platform and its many capabilities. The most important—and most rewarding—role he fills is as EDX liaison between the product's users and its developers, or, as Chad described it, "between the researchers and the IT guys." EDX is a living creation that adapts to meet the needs of its users, so the role of liaison is essential. "I take what the researchers want and package it so the developers can work with it," Chad said. "It's rewarding to be able to build tools that directly facilitate researchers' needs."

What are his favorite features of the system? Chad cites EDX's unique capacity to enable document sharing between internal and external collaborators. "Researchers wanted to be able to share private data with their external collaborators so we built Collaborative Workspaces." He's also enthusiastic about the newly released Slate functionality for Collaborative Workspaces. Slate will allow members of a Collaborative Workspace to create their own custom page content.

Chad is optimistic about the future of EDX, which started as a few basic tools for NETL researchers and is now taking on even bigger challenges. Every week, Chad gives multiple demonstrations of the system and its features to researchers all over the country, including collaborators at other National Labs and DOE Headquarters. He sees real potential for EDX to go beyond NETL. It's uncharted territory, but whom better to have on hand than a GIS expert?

Contact: Chad Rowan




*Chad Rowan demonstrates how to use the EDX website.*

# NETL's In-House Research Program:
## Advanced Gasification

About 75 percent of any product's manufacturing costs is committed early in the development process, during the conceptual-design stage. NETL offers a suite of computation-fluid-dynamics models that helps developers reduce manufacturing costs for gasifier systems, and optimize how the systems perform. The open-source suite, called Multiphase Flow with Interphase eXchanges (MFIX), has become the standard test for comparing, implementing, and evaluating multiphase flow constitutive models—that is, models that show how a material responds to the force of another material.

Researchers supporting NETL's Advanced Gasification Program are constantly improving MFIX. In addition, they are seeking out their own new concepts for gasification and performing their own studies of how materials interact during gasification. The researchers' tasks are to:

- Develop, speed up, and validate large-scale MFIX models (including the Two-Fluid Model, the Discrete Element Model, and Multiphase Particle-in-Cell) that can be used to study advanced gasification technologies.
- Generate lab-scale data for developing and validating models using velocimetry (speed of a fluid) and standard measurement techniques.
- Promote novel gasification concepts that can make coal gasification less costly, increase the overall efficiency of gasification systems, and reduce emissions—by using computational methods, performing literature studies, running laboratory experiments, and assessing the cost-effectiveness of new gasification technologies.
- Conduct laboratory experiments to determine how materials interact during gasification, find ways to extend the service life of refractory (heat-resistant) materials, and keep ash particles from sticking together during gasification.

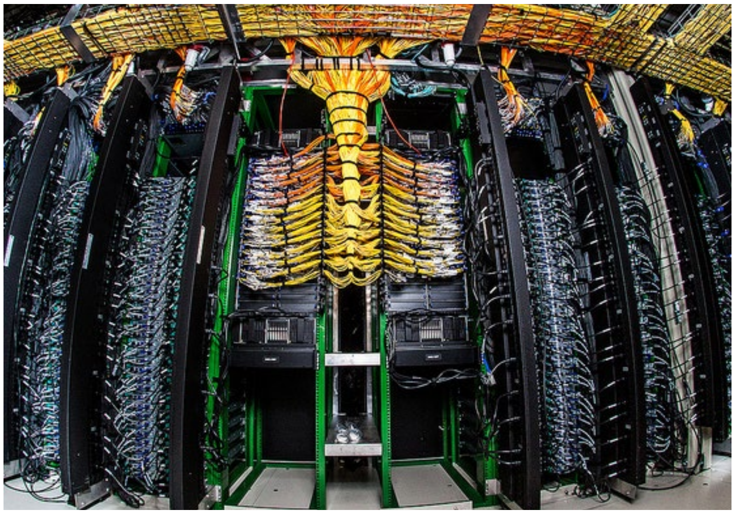
For more information on gasification models, contact Dr. William Rogers. To learn more about new gasification concepts, contact Dr. Dushyant Shekhawat. Contact James Bennett to discuss NETL's research into material interactions.

FUNDAMENTAL FUN

# What Is Big Data?

"Big Data" is a catch-phrase that has recently gained prominence, from business and industry to academia and research. Large and complex datasets are being assembled from multiple eclectic sources, from remote sensing instruments to social media, and are massive and often unstructured. Three characteristics define big data: 1) the volume of information involved; 2) the velocity at which the information is gathered; and 3) the diversity of data sources and formats.

The concept of big data is multi-faceted, conjuring different connotations based upon who the end user is and what the data are used for. For instance, numerical modelers and simulators tend to conceive of big data in terms of computing power required for the simulation–can it be performed on a standard computer, or will it require a supercomputer? Earth systems scientists tend to think of big data in terms of streaming datasets involving information being collected at high velocity. Analytical scientists consider big data in terms of the size of the datasets they are dealing with, data produced over months or years of research to be mined for valuable insights. But what every scientist gains by undertaking big data projects is, simply put, new understandings of relationships in the data currently hidden by the separation of the various data streams.



Handling big data can be complicated; the volume and velocity stress information technology infrastructure. In addition to affecting storage arrays, data management, and analytics tools, big data can pose a problem for server infrastructure, storage networks, data networks, and archiving solutions. However, as big data continues to prove essential in our changing world, new tools and techniques for dealing with it are evolving and emerging. NETL's EDX system is now developing methods to incorporate big data storage and analytical features into the platform in support of NETL's R&D needs.

# APPLAUSE

## Patent Issued

*Apparatus and method for solid fuel chemical looping combustion*, **Dr. Ranjani V. Siriwardane** (DOE/NETL); and **Justin M. Weber** (DOE/NETL), 9,004,911, issued December 9, 2014.

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## Kudos!

**Dr. DeNyago Tafen**'s paper entitled "First-principles-based kinetic Monte Carlo studies of diffusion of hydrogen in Ni–Al and Ni–Fe binary alloys" (*Journal of Materials Science* (2015) 50:3361-3370) was selected as the May finalist for the 2015 Cahn Prize. The Journal of Materials Science Robert W. Cahn Best Paper Prize (the "Cahn Prize") recognizes a truly exceptional original research paper published in the journal in a particular calendar year. Each month the Editors select a paper published in that month's issues via a rigorous nomination and voting procedure. The winning paper is then selected from the twelve finalists by a separate panel of distinguished materials scientists. All the twelve finalists will be recognized and the winner will be announced at the 2015 Fall MRS Meeting in Boston, MA.

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The Pittsburgh Business Times "Energy Leadership Awards" honor individuals and organizations for their efforts in advancing energy business interests in western Pennsylvania. NETL had two winners of this award. **Dr. Barbara Kutchko** received this award for her work in ensuring that oil and natural gas resources in volatile environments, including western Pennsylvania's Marcellus shale and U.S. offshore resources, will be produced sustainably and with minimal environmental impact. **Dr. Shiwoo Lee** received this award for his one-step cathode infiltration technique, which benefits both the coal and natural gas industries in western Pennsylvania and potential fuel cell manufacturers in the Pittsburgh region. These NETL award winners were recognized in the May issue of the Pittsburgh Business Times.

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