

# Research news

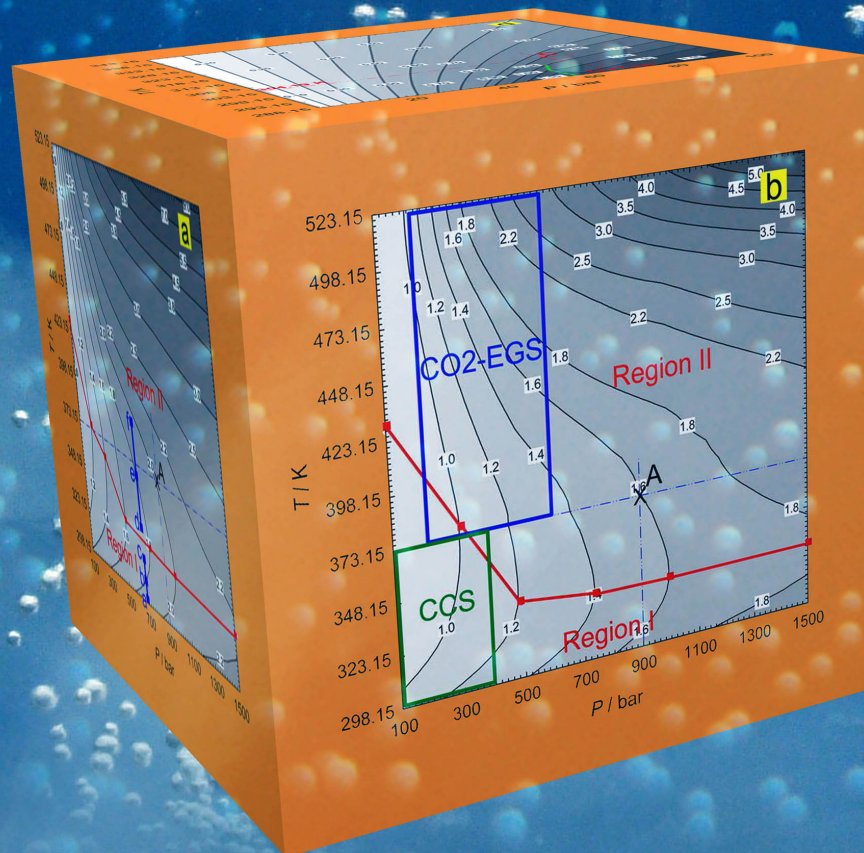


June 2015, Issue 9

FEATURE STORY:

## Experiments and Models Help Predict CO<sub>2</sub> Solubility in Brines

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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.

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# EXPERIMENTS AND MODELS HELP PREDICT CO<sub>2</sub> Solubility In Brines

Carbon dioxide (CO<sub>2</sub>) can be injected into geologic formations to improve oil and gas recovery, to be used as a medium to extract energy from geothermal systems, or to be safely stored to reduce emissions to the atmosphere. NETL's research on CO<sub>2</sub> storage focuses on developing technologies and analyses to understand and improve injection operations and containment, increase geologic reservoir storage efficiency, and prevent and mitigate unwanted migration of CO<sub>2</sub> (see article "Novel Techniques for Field Measurement of CO<sub>2</sub> in Groundwater," page 4). The results of this research will help ensure that CO<sub>2</sub> can be geologically stored efficiently, that stored CO<sub>2</sub> does not leak to the atmosphere where it can contribute to global climate change as a greenhouse gas, and to identify and manage potential technical risks associated with large-scale, long-term storage.

Saline formations, which are present in many parts of North America, represent

an enormous potential resource for geologic CO<sub>2</sub> storage. These porous layers of rock are saturated with brine—sea water that accumulated in the formation and became concentrated over many millions of years. As CO<sub>2</sub> is injected into a saline formation, it contacts and gradually displaces brine from pores in the formation rock. The CO<sub>2</sub> is trapped by overlying and adjacent low-permeability barriers, immobilized in small pores or dissolved in the brine that it contacts. Over time, dissolved CO<sub>2</sub> may interact with the geologic storage formation to dissolve some rocks and form minerals called carbonates. Dissolution of CO<sub>2</sub> into brine influences the amount of CO<sub>2</sub> that can be stored, the rate at which CO<sub>2</sub> can be injected, and the ability of injected CO<sub>2</sub> to form a more stable compound that helps keep it underground.

Dissolving CO<sub>2</sub> in brine impacts engineered geologic systems, including the formation rock, formation fluids like oil and gas, the wellbore, and cement

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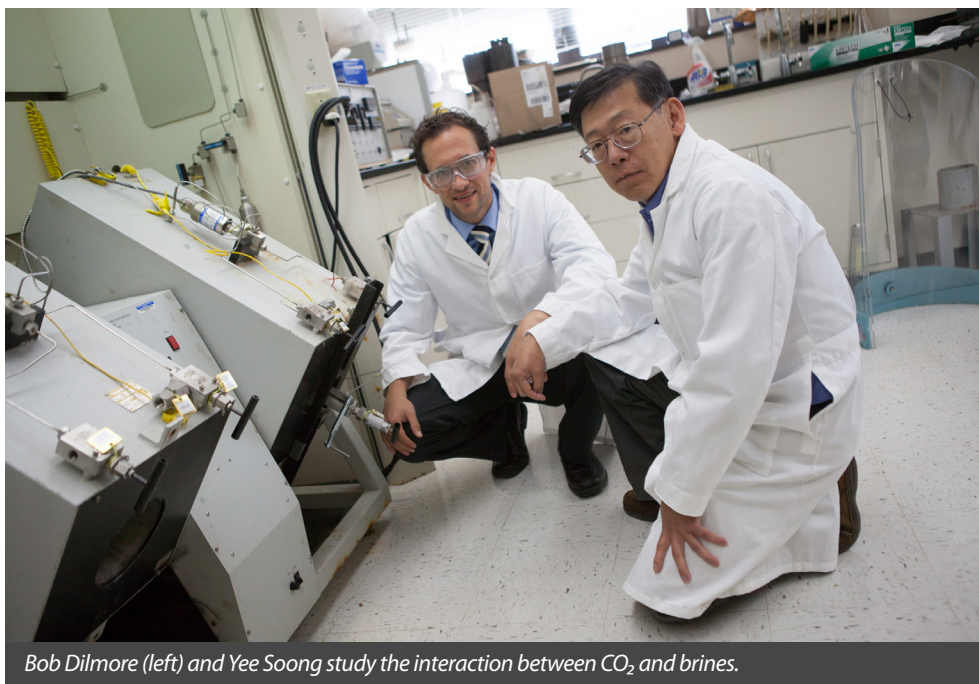
**Cover image**  
CO<sub>2</sub> solubility in brines.



that supports the wellbore. “As the CO<sub>2</sub> dissolves in the brine, it can change the rate and extent of mineralization and corrosion in these systems,” Research Engineer **Robert Dilmore** explained. NETL researchers are examining how CO<sub>2</sub> interacts with different engineered and geologic components of the system and developing models that accurately predict that behavior.

As one aspect of that effort, NETL researchers collaborated with researchers at Pennsylvania State University (Professor Serguei Lvov) and Salem State University (Salem, MA; Doug Allen, [ORISE](#) faculty researcher and professor of geology). The team made laboratory measurements of CO<sub>2</sub> solubility in brines and developed models to describe how much CO<sub>2</sub> can dissolve in brine over a range of temperatures, pressures, salinities, and brine compositions.

Experimental CO<sub>2</sub> solubility measurements were made at temperatures up to 150 °C, pressures up to 3,000 pounds per square inch (psi), and in brines containing one or more salts. These measurements were made using Penn State University’s specially designed, corrosion-resistant continuously stirred autoclave reactors

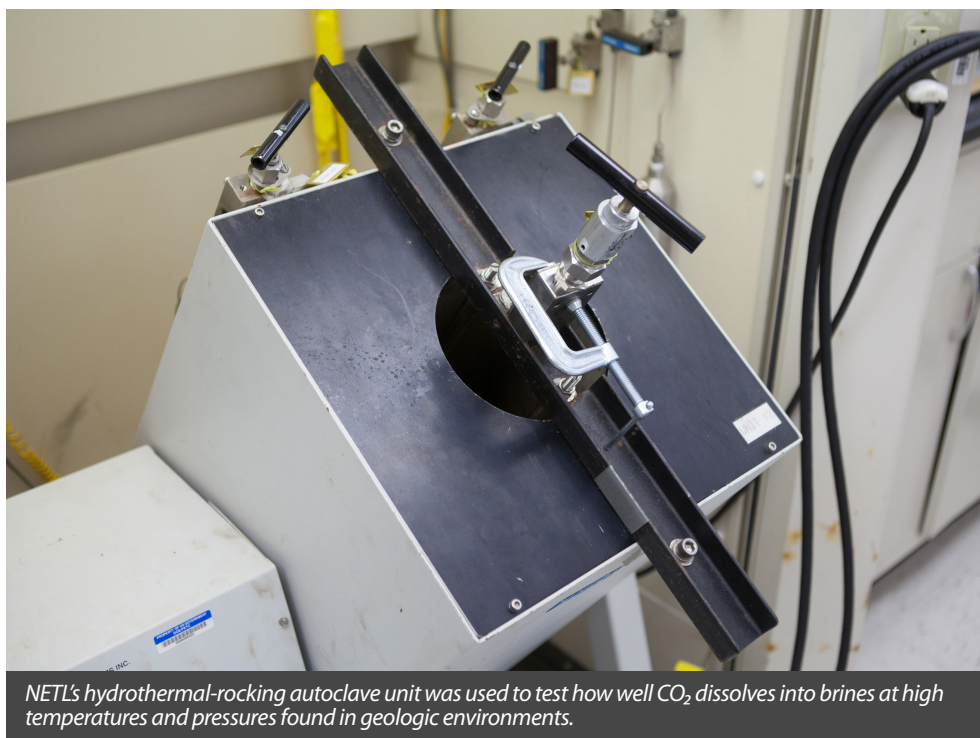


Bob Dilmore (left) and Yee Soong study the interaction between CO<sub>2</sub> and brines.

and NETL’s hydrothermal-rocking autoclave test unit. NETL’s unit rocks back and forth rather than stirring a sample to mix it, reducing the sample’s exposure to metal parts that could corrode. These new data were combined with others reported in peer-reviewed literature from the past 125 years, and the resulting database was used to develop improved models of the solubility of CO<sub>2</sub> in brines in a variety of geologic conditions.

Generally, the new models were in agreement with previously developed models on general trends in CO<sub>2</sub> solubility related to brine’s salinity, temperature, and pressure. Less CO<sub>2</sub> can dissolve in higher salinity brine, less CO<sub>2</sub> can dissolve at higher temperatures, and more CO<sub>2</sub> can dissolve at higher pressures. However, the new model shows a minor deviation from that general trend: as temperature increases, the liquid phase decreases monotonically—for a certain temperature range, the liquid phase didn’t increase. The model also demonstrates improvements over CO<sub>2</sub> solubility predictions compared to previously published models, in moderate to highly saline brines and at mild to moderate CO<sub>2</sub> storage and enhanced oil recovery environmental conditions. These results can be applied to improve characterization of CO<sub>2</sub> injection and long-term storage performance. Results of these efforts have been published in articles appearing in peer reviewed literature, including [Environmental Science & Technology](#), [Geochimica et Cosmochimica Acta](#), and [AIChE Journal](#).

Contact: [Robert Dilmore](#), [Yee Soong](#)



NETL’s hydrothermal-rocking autoclave unit was used to test how well CO<sub>2</sub> dissolves into brines at high temperatures and pressures found in geologic environments.



# Novel Techniques for Field Measurement of CO<sub>2</sub> in Groundwater



A water sample is being injected into the carbonation meter for testing.

If CO<sub>2</sub> were to leak from a geological storage site, it could migrate into and impact overlying groundwater aquifers, some of which supply drinking water. To spot leaks early and protect the water supply, sensitive and accurate methods are needed to measure CO<sub>2</sub> concentrations in the field.

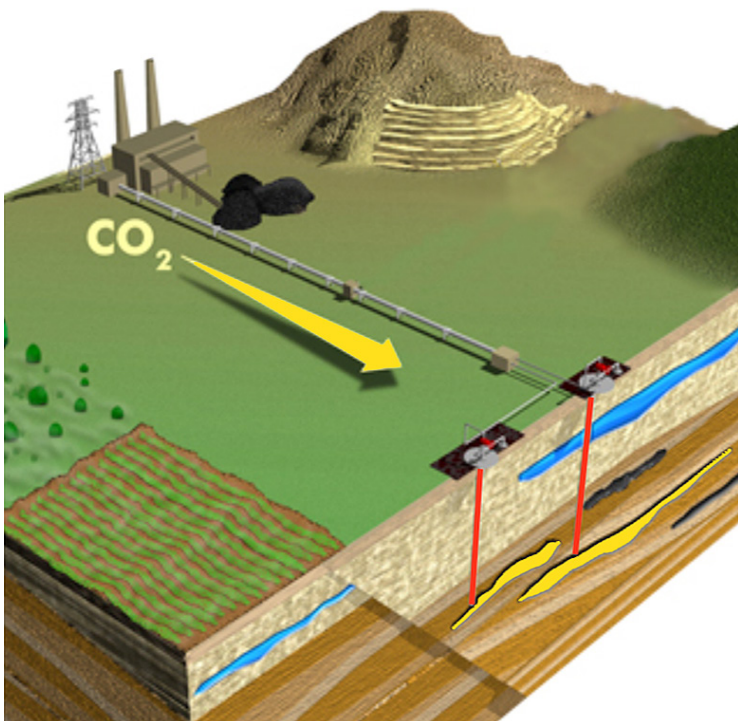
NETL successfully tested two different methods of CO<sub>2</sub> detection at CO<sub>2</sub> natural analog sites, including thermal springs and coal mine drainage sites, which are

naturally elevated in CO<sub>2</sub> but provide easier access for sampling than deep geological storage wells. One method, previously used only by the carbonated beverage industry, employs a carbonation meter to expand a sealed volume of water, via a process called "multiple volumetric expansion." This technique releases gases from solution in a controlled manner based on their relative ability to be dissolved. The resulting changes in temperature and pressure allow the CO<sub>2</sub> concentration to be accurately determined.

A second method uses a non-dispersive infrared detector to identify CO<sub>2</sub> that escapes from the water and through a waterproof but gas-permeable membrane.

Further testing of the two methods is being planned for this summer, with the goal of measuring CO<sub>2</sub> concentrations in groundwater monitoring wells associated with a geologic storage site.

Contact: [Hank Edenborn](#), [Christina Lopano](#)



CO<sub>2</sub> injection into deep formations (yellow). Other deep formations (black) and groundwater aquifers (blue) may be monitored for potential CO<sub>2</sub> migration.

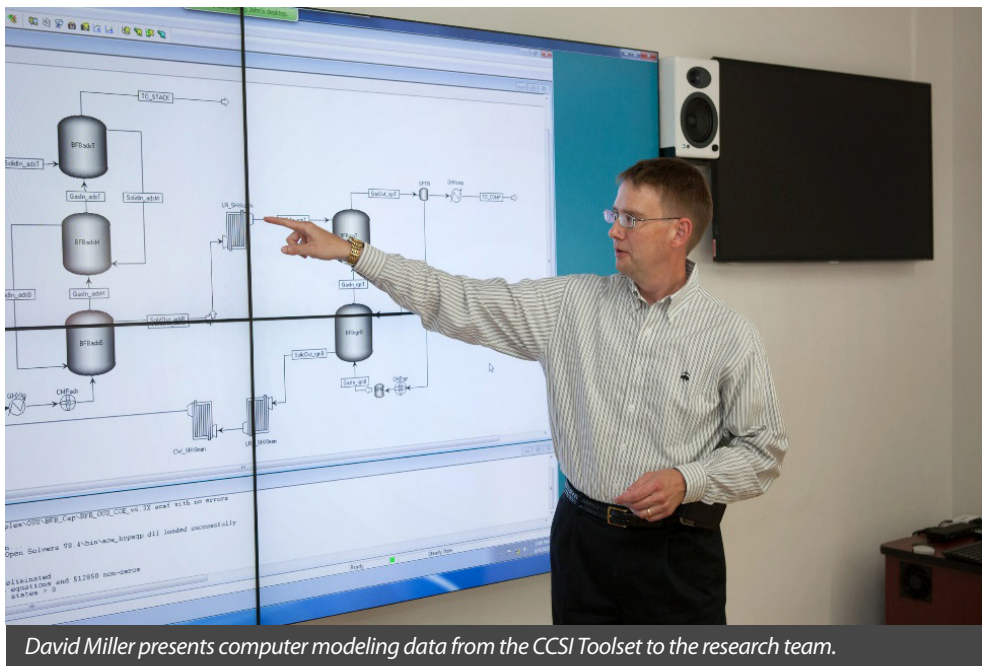
# New Tool Predicts Behavior of Materials Used in CO<sub>2</sub> Capture Processes

The more confidence industry has in the safety, economy and efficiency of new technologies that capture CO<sub>2</sub> from fossil fuel-burning processes, the more likely those innovations can be deployed to remove greenhouse gases from emissions.

A team of researchers from the NETL-led [Carbon Capture Simulation Initiative \(CCSI\)](#) developed a modeling tool to predict the behavior of materials used in solvent-based CO<sub>2</sub> capture processes. This latest addition to the CCSI Toolset provides a higher level of confidence in the projected performance of carbon-capturing solvent systems on fossil fuel burning plants.

The new tool works by quantifying uncertainties in property data that could have performance-altering implications. Using multiple computer experiments to sample uncertain model parameters is the most common approach to studying the effects of parametric uncertainty on model predictions. The more thoroughly sources of uncertainty are identified and scrutinized, the greater the opportunity to increase confidence in the results of the simulations, reducing technical risk during scale up. This process of reducing uncertainties in simulations is “uncertainty quantification.”

Researchers must have a detailed understanding of how materials used in a solvent-based CO<sub>2</sub> capture process will behave when scaled up to full operation, according to **David Miller**, the technical director of CCSI. “The physical properties, thermodynamics, and kinetics of the



David Miller presents computer modeling data from the CCSI Toolset to the research team.

materials being used to capture CO<sub>2</sub> need to be well understood to accurately predict the way a process is going to behave when scaled up,” he said.



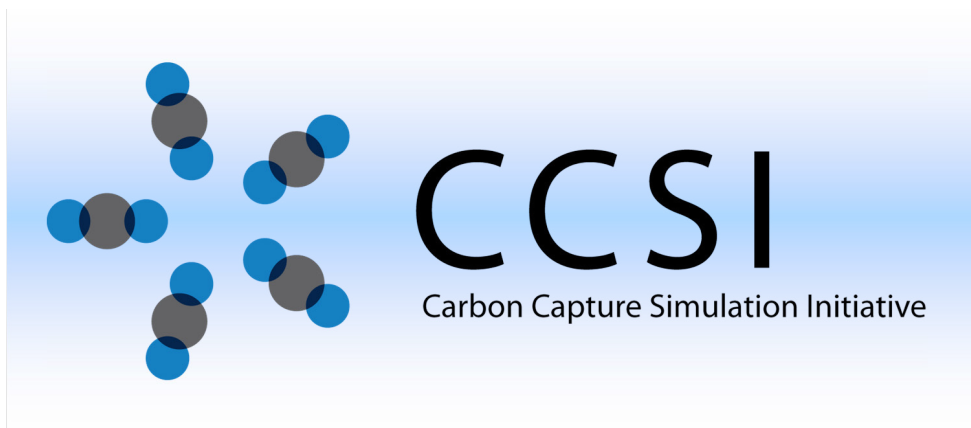
He added that the newly developed tool uses experimental data to assess physical properties such as viscosity, density, surface tension, heat capacity, and diffusivity. To account for model uncertainties and data uncertainties that occur because of routine experimental or measurement errors, the new process

applies a Bayesian methodology—a statistical method based on Thomas Bayes’ probability theorem involving prior knowledge and accumulated experience—to arrive at improved model predictions with quantified confidence.

“Bayesian calibration is certainly not new,” Miller said. “But it has never been applied to properties models of carbon capture systems before. The underlying computational framework will enable the development of rigorous models with quantified uncertainties for a variety of solvent-based carbon capture systems. That’s important because our current knowledge about typical chemical solvents that have high potential for application to post-combustion CO<sub>2</sub> capture systems is incomplete.”

Miller said the new approach will be incorporated into the next generation of the CCSI Toolset to be released in October. The CCSI Toolset provides end users in industry with a comprehensive, integrated suite of scientifically validated models, with uncertainty quantification, optimization, risk analysis, and decision-making capabilities.

Contact: [David Miller](#)





# New Capability Takes Sensor Fabrication to a New Level

Operators must continually monitor conditions in power plants to assure they are operating safely and efficiently. Researchers on NETL's Sensors and Controls Team can now fabricate prototype optical sensors that demonstrate superior properties in comparison to traditional sensors using a new laser-heated pedestal growth (LHPG) system. According to NETL researcher **Michael Buric**, "The new sensors have broader functional temperature ranges, increased durability, and reduced cost. Sensors produced using LHPG will be capable of operating in the high temperature and harsh environments associated with advanced power systems."

LHPG is a crystal growth technique that reforms bulk high temperature-resistant materials, such as sapphire or YSZ (yttrium stabilized zirconium), into single-crystal optical fibers. The technique produces optical fibers with very high melting temperatures for use as sensor substrates. The LHPG system enables researchers

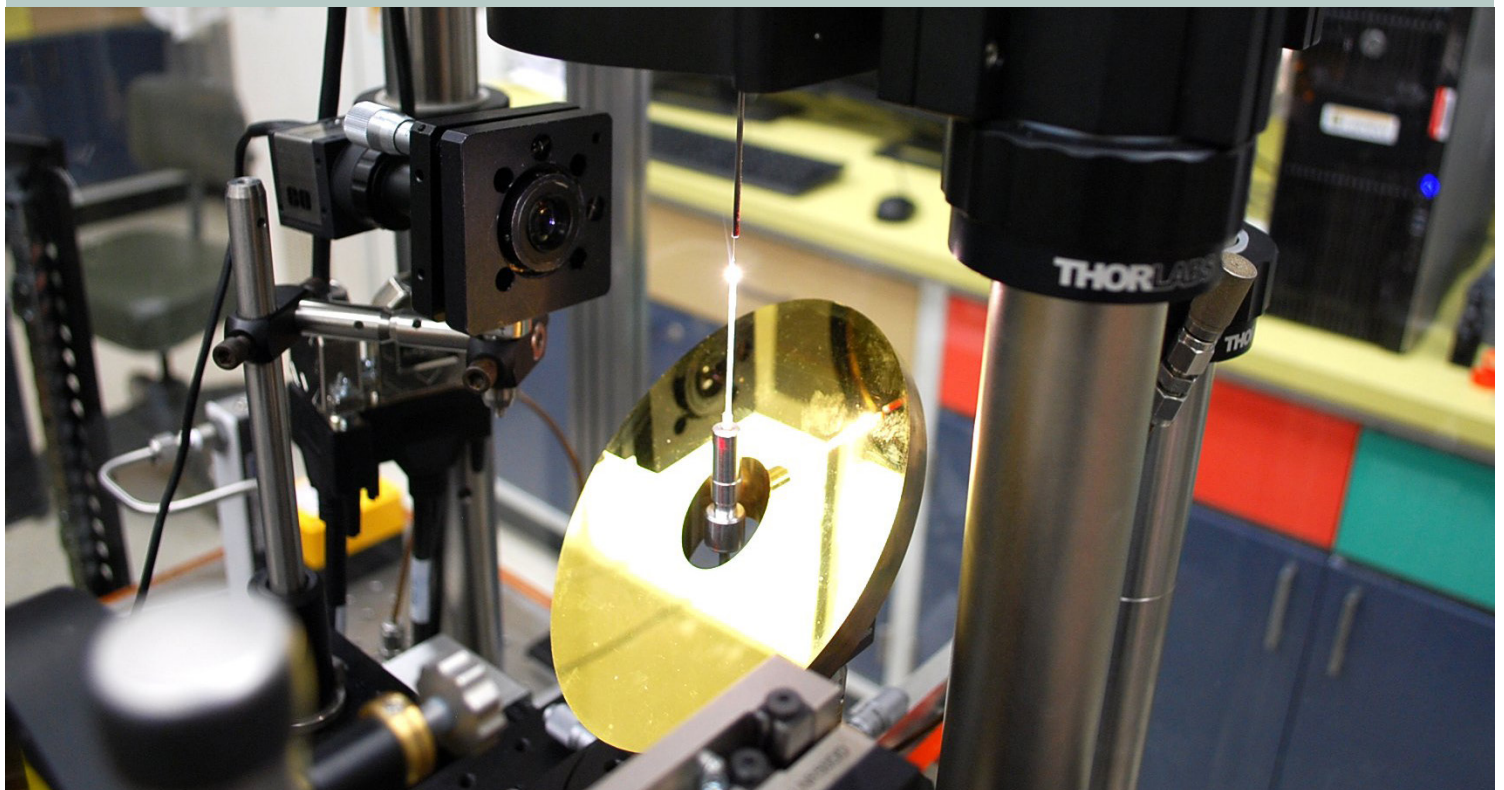
to precisely control crystal growth, and to incorporate novel sensor materials with fiber-substrates during the growth process. The ability to control fabrication parameters along with high temperature-resistant materials generates optical fiber sensors with improved measurement sensitivity and durability. The optical fibers developed at the new facility will be incorporated into fiber sensor assemblies and evaluated for functionality under high temperature and pressure conditions. The materials that demonstrate the most promising performance characteristics will be further evaluated in various sensing configurations.

Optical fiber-based sensors offer distinct advantages including broadband wavelength and compatibility, and resistance to electromagnetic interference. They also eliminate electrical wires and contacts, which are commonly associated with sensor failure. Additionally, fiber optic sensors are compatible with embedded, remote, and distributed sensing technologies.

Innovative process control systems capable of functioning in the extreme environments of conventional and future fossil fuel-based power generation systems will play a key role in improving efficiency while reducing carbon dioxide (CO<sub>2</sub>) emissions.

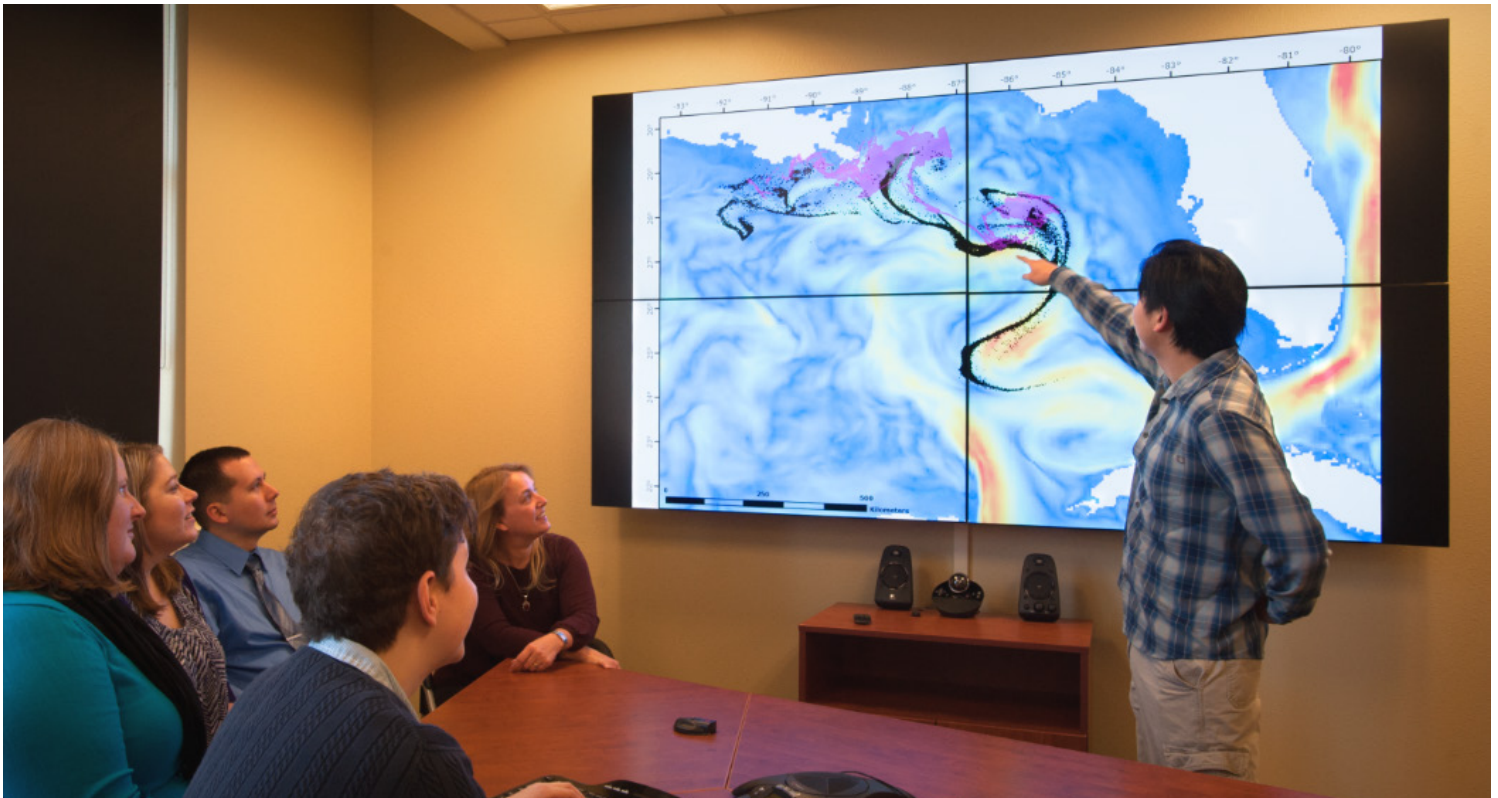
Advanced sensor materials will enable continued use of our coal resources to improve U.S. economic competitiveness while providing global environmental benefits through reduced greenhouse gas emissions. The sensors developed using LHPG could also be applied to process monitoring and control for other energy systems, including solid oxide fuel cells, gas turbines, boilers, and oxy-fuel combustion. [Other research](#) at NETL is expanding the application of fiber optic-based sensors for use in subsurface monitoring including unconventional, deep, and ultra-deepwater oil and gas resource recovery and CO<sub>2</sub> storage.

Contact: [Michael Buric](#)



*A sapphire rod being melted in the Laser Heated Pedestal Growth system. A sapphire seed crystal is being lowered onto the molten sapphire rod to begin the growth of a single-crystal sapphire fiber.*

# GAIA and the NETL Supercomputer Create Cutting-Edge Modeling Facility



*In the NETL GAIA and Visualization Centers, scientists share simulations and data, create geospatial analysis tools, and benefit from research collaborations.*

As hydrocarbon exploration pushes into more remote and extreme environments to meet increasing energy needs, it is vital to keep developing technology and risk assessment methods in order to keep pace with the growing energy demand. In order to support risk reduction efforts, spatio-temporal and geostatistical approaches to technology development are being used to detect data trends, reduce geologic uncertainty, identify knowledge gaps, and evaluate environmental risks for carbon storage and hydrocarbon-related systems such as geologic carbon storage, and conventional and unconventional hydrocarbons. At NETL, top-of-the-line facilities enable the advanced computational capacities and collaborative workspaces needed to create the cutting-edge modeling tools.

The Geoscience Analysis, Interpretation, and Assessments (GAIA) computational facilities at NETL allow scientists at the Albany, OR, Morgantown, WV,

and Pittsburgh, PA, sites to work collaboratively. These scientists use the GAIA facilities to engage in collaborative research with partners in academia and at laboratories in the DOE system. GAIA provides a workspace that enables scientists that are spread out over the country to connect through high-powered computers that can handle the advanced visualizations and statistical and analytical software packages needed to develop spatio-temporal and geostatistical tools.

In GAIA, the Energy Data eXchange (EDX) allows users to access data and collaborate on research while developing geospatial models. Once those products and tools are fully developed, they are often made available on EDX. Some of the most used tools on EDX, like BLOSOM and GeoCube, were created as part of research conducted by users in the GAIA facilities. Through GAIA, researchers can visualize, interpret, analyze, and model spatial data sets obtained from the lab or

the real world, and then through EDX, they can grant a platform to the tools that they have developed.

NETL is also home to a supercomputer, one of the world's largest high-performance computers, along with advanced visualization labs serving the organization's research and development needs. A unique and collaborative tool tailored for engineering calculations in support of fossil energy research, the supercomputer progresses NETL's mission by applying complex model simulations for advanced energy technology development. Visualization labs for the supercomputer are installed at each of the three NETL sites and provide a dedicated space for researchers to engage in collaboration and simulation work.

Contact: [Kelly Rose](#) (GAIA), [Bill Rogers](#) (NETL supercomputer)



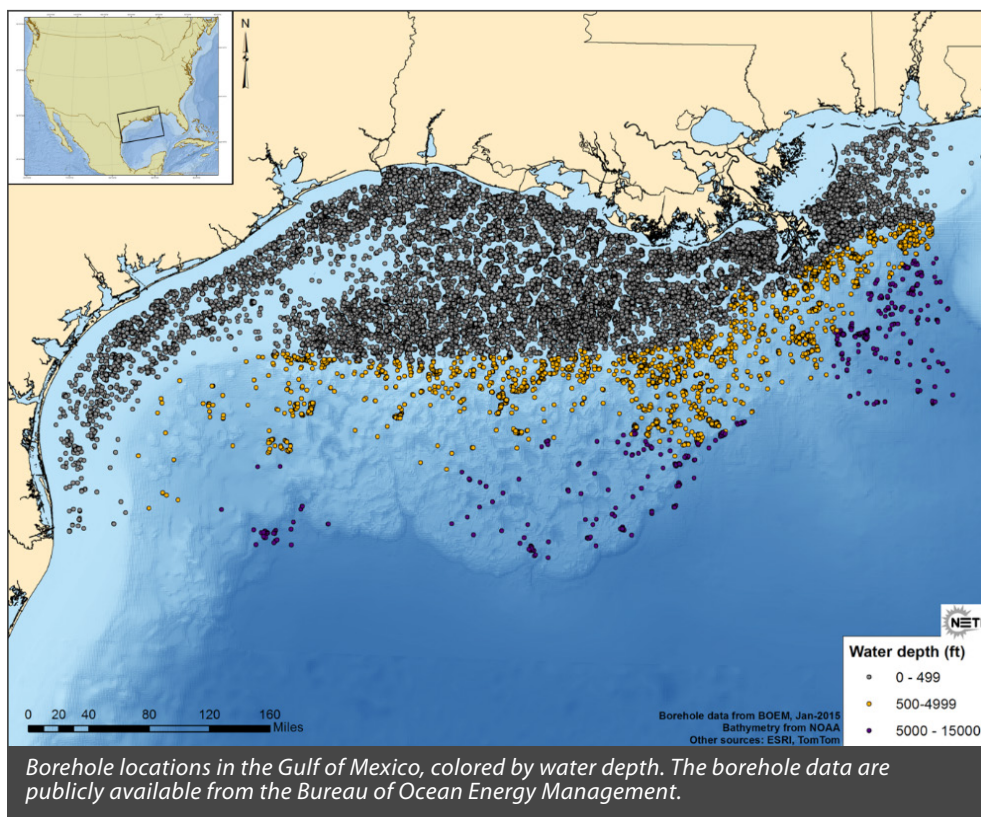
# Combating Offshore Drilling and Production Risks

For decades, the Gulf of Mexico (GOM) basin energy reserves have been an important domestic source of natural gas and crude oil. These resources will continue to play a critical role in meeting U.S. energy needs, provided they're produced while effectively addressing environmental concerns. Science-based decision making, risk reduction, and identifying technology gaps are essential to responsibly developing offshore hydrocarbon resources.

Recognizing this need, NETL's Geology & Geospatial Team compiled relevant peer-reviewed and open-source publications, as well as publicly available databases, with information on the GOM's deep and ultra-deepwater basins. The results were recently [published](#) as a comprehensive review article of the GOM's subsurface petroleum system.

Because drilling is relatively recent in deepwater and ultra-deepwater regions, fewer datasets are available for these areas than for the continental shelf. Even so, study author and Research Scientist **Corinne Disenhof** emphasized that much information is available. "Proprietary data sets and resources are often coveted for the information they can offer, but the breadth and range of publicly available data and published literature about these systems offers significant opportunities to advance the public state of knowledge about the subsurface GOM hydrocarbon system, particularly in deep water and the deep subsurface."

As GOM offshore hydrocarbon development ventures into deeper waters and more technically challenging subsurface environments, the tools to evaluate and reduce risks



Borehole locations in the Gulf of Mexico, colored by water depth. The borehole data are publicly available from the Bureau of Ocean Energy Management.

continue to evolve along with our understanding of potential drilling impacts. According to Disenhof, "The information the team assembled will be of value to a range of stakeholders, including industry, regulators, and researchers, to identify solutions to gaps in knowledge and technology related to offshore exploration, production, and operations in the GOM." NETL uses the data summary to [support risk assessment models and predictions](#) such as those from the Offshore Integrated Assessment Model.

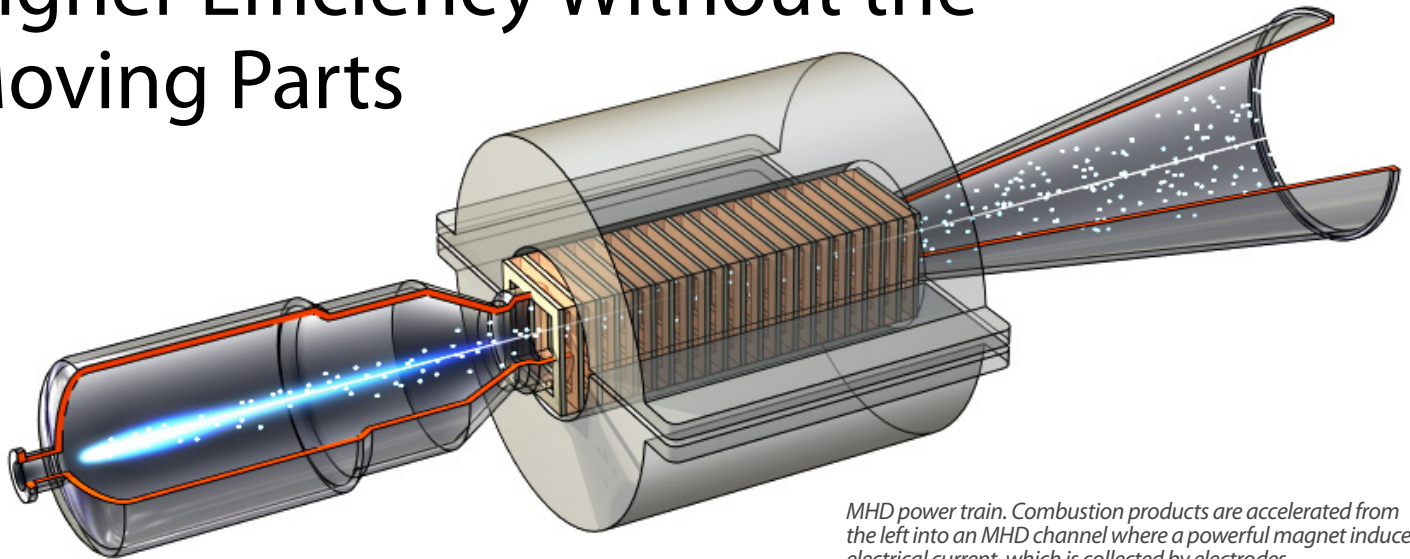
The team is currently developing a centralized database to house relevant GOM data and information, including new interpretations and analysis methodologies developed by NETL. Once completed, this Subsurface Databook will be incorporated into NETL's [Energy Data eXchange](#), an online coordination and collaboration

platform available to the NETL research community and their strategic partners. The Databook will join other EDX tools such as [Geocube](#), an EDX web mapping tool that helps users find and access publicly available GOM data. The Geology & Geospatial Team's work directly supports the mission of NETL's [Offshore Research Program](#). Team members include Corinne Disenhof, **MacKenzie Mark-Moser**, **Kelly Rose**, **Roy Miller**, and **Steve Galer**.

Contact: [Corinne Disenhof](#)



# Higher Efficiency Without the Moving Parts



*MHD power train. Combustion products are accelerated from the left into an MHD channel where a powerful magnet induces electrical current, which is collected by electrodes*

**D**irect Power Extraction (DPE) refers to the conversion of the thermal or kinetic energy in a fluid, such as the gas stream in a power plant, directly into useable electrical power. By avoiding an intermediate mechanical energy conversion step (such as the movement of turbine blades), power generation efficiencies can be extended beyond what is currently possible.

One approach for achieving DPE is through a device called a magnetohydrodynamic generator. Magnetohydrodynamics (MHD) refers to the forces and properties of electrically conductive fluids, such as plasmas, in a magnetic field.

**Rigel Woodside**, NETL research general engineer and research lead for DPE, explained the concept of MHD power generation, “You’re removing the turning mechanical blades. The moving part then is the actual gases, which are made to be electrically conductive. Essentially, it’s an electromagnetic turbine.”

MHD generators can be operated at very high temperatures, which means they can be highly efficient. The high temperature capability of MHD generators is particularly synergistic with the oxy-fuel approach to carbon capture, which can produce high-temperatures. Oxy-fuel combustion uses pure oxygen, rather than air, to burn fuel. As a result, oxy-fuel exhaust products consist almost exclusively of water and CO<sub>2</sub>, enabling easy removal of water and leaving a near pure CO<sub>2</sub> stream for capture.

NETL’s DPE task objectives are to generate useful engineering data sets, simulation tools, materials, and new concepts to further the prospects of DPE technology. The task is presently focused on challenges that are unique to achieving DPE as the primary fuel-to-electricity conversion system. Below are examples of the DPE team’s current investigations:

- **Engineering Data Sets**—The NETL research team is predicting the electrical conductivity of “seeded”—seeded meaning there is an addition of small amounts of material to enhance the number of free electrons—oxy-fuel products in motion, and then compiling data on the properties of these products.
- **Simulation Tools**—Researchers developed and implemented a one-dimensional computational fluid dynamics code for investigating MHD generator design and simulation. NETL plans to eventually release this code for general public use, as there is currently no other commercial or research code available with this capability. Currently, researchers are using the NETL code to design a utility-scale MHD generator for use in analyzing DPE systems.
- **Materials**—Researchers are investigating materials for MHD electrodes and have fabricated candidate ceramic electrodes. Their next task is to assess the candidate materials and evaluate how the electrode materials interact with seed

materials, since these interactions will be an important consideration for selecting materials appropriate for the area of conducting fluids, or “channel.” Electrodes allow electrical power to be drawn from the electrically conductive plasma in an MHD generator.

- **New Concepts**—Researchers are developing a technique to assess allowable electrical stresses and measure the induced magnetic fields outside the channel. This information will enable validation of predictive models and help establish material-dependent critical current densities. A critical current density represents a maximum value that can be achieved in the generator without arcing, which damages the electrodes.

NETL’s current DPE research is fairly fundamental, and Woodside recognizes that there are many ways the physics of MHD might be used in power generation. The biggest driver for NETL’s exploration of DPE is to limit carbon emissions from fossil fuel power plants. He explained that “While the production of oxygen has traditionally been the most expensive aspect of the oxy-fuel approach to carbon capture, DPE flips this around and allows for oxygen production to be made the greatest strength of carbon capture technology that can enable highly efficient, zero-emission plants.”

Contact: [Rigel Woodside](#)

# NETL Honors Former Lab Director in Celebration of His Centennial Birthday



Wender's work with organometallic intermediates—the study of chemical compounds containing at least one bond between a carbon atom of an organic compound and a metal—led researchers to discover a reaction that helped further develop Fischer-Tropsch synthesis. A Wender-led team's organometallic breakthroughs on hydrocarbons in the laboratory attracted the praise of [Linus Pauling](#), who founded the fields of quantum chemistry and molecular biology research. He wrote to Wender's team to congratulate them on their discoveries.

While working at BERC, Wender earned a Ph.D. in chemistry from the University of Pittsburgh, and in 1953, he was selected by Storch to head the organic chemistry section of the lab, working with synthesis gas and dehydrogenating coal using a palladium catalyst to make hydrogen for energy use.

Eventually, Wender took the helm as director of BERC—a position he initially rejected because of his passionate dedication to research. However, he overcame that reluctance and ushered in a prolific period in the facility's research history from 1972 through 1979—a time when money was being poured into energy research because of the [energy crisis](#).

Natural gas shortages during the cold winter of 1976–1977 prompted Wender's researchers to investigate ways to tap unconventional natural-gas reservoirs that could yield natural gas in large quantities. Researchers began mapping gas-bearing rock formations—like shales and tight sandstones—to help identify physical and chemical characteristics, the amount of natural gas they contained, underground fracture patterns, and other characteristics that could aid in development.

As BERC evolved into the Pittsburgh Energy Technology Center (PETC), Wender recognized that reducing

coal's contributions to air pollution to comply with new national standards was paramount to allowing the nation to continue to make use of its substantial domestic coal resources. Under his leadership, researchers focused on fluidized bed combustion, coal gasification, integrated gasification combined cycle technology, substitute natural gas and synthetic liquid fuels made from coal, and other technologies designed to make a significant energy impact. Wender's expertise was in demand elsewhere in the federal government, and he eventually left PETC to tackle a series of critical assignments in Washington. He followed this work with educating the next generation of chemists and energy researchers at the University of Pittsburgh.

Wender made outstanding contributions throughout his career, as an innovative researcher, energy leader, and dedicated educator. His work resulted in more than 200 papers, five edited books, and 11 patents. His work attracted a wide range of recognition. In addition to the Storch Award, he received accolades from the Secretary of Energy including one "in recognition of advancing fossil energy technology through highly innovative research on catalytic conversion of syngas to fuels and chemicals, coal liquefaction, and decisive guidance and inspirational leadership in shaping research programs in government, academia, and industry." The University of Pittsburgh's Department of Chemistry named him a Distinguished Alumni in 2002 for his impressive career and contributions.

NETL is pleased to wish Dr. Wender all the best as he celebrates this milestone birthday and to commemorate his outstanding career in energy research. Happy birthday Dr. Wender!

In a rich, productive life of research, teaching, and discovery, Dr. Irving Wender has been on a remarkable 100-year journey that took him from humble beginnings in the Bronx, NY, to atomic bomb research in secret labs of Chicago; energy research laboratories and university classrooms of Pittsburgh; and the halls of government in Washington, D.C.—all in pursuit of scientific advancements that continue to set high standards of excellence for the generations of scientists who follow in his footsteps.

After his discharge from the U.S. Army where he worked on the Manhattan Project, Wender learned that the U.S. Bureau of Mines' Pittsburgh Experiment Station in Bruceton, PA—an NETL predecessor organization—was looking for researchers to work on an energy project. He wrote to Dr. Henry Storch, who headed the Station, and Storch offered Wender a research position. In 1946, the Pittsburgh Experiment Station became the Bruceton Energy Research Center (BERC).

Wender worked on reactions that would provide insight into [Fischer-Tropsch](#) synthesis, a process first developed by German scientists to convert carbon monoxide and hydrogen into liquid hydrocarbons like low-sulfur diesel fuel. The United States was attempting to duplicate the process.



# NETL's In-House Research Program: Carbon Capture Simulation Initiative

Commercial deployment of a new technology typically takes 20 to 30 years. An effective method of reducing the time and cost to develop new technology is to apply computer-based tools to more rapidly identify promising concepts, troubleshoot new designs, and quantify the sources and effects of uncertainty to guide experimental testing and larger-scale demonstration. Through the Carbon Capture Simulation Initiative (CCSI), researchers from NETL have teamed with other national laboratories, industry, and academia to develop and validate a suite of computational tools and models, called the CCSI Toolset, with the goal of accelerating deployment of promising carbon capture technologies. NETL and its partners are further developing the CCSI Toolset by executing the following tasks:

- Continue to develop and test uncertainty models in the CCSI framework to include new capabilities, such as optimization under uncertainty and an improved user interface that will facilitate execution of the various modules in the toolset.
- Develop detailed, customized, and validated versions of solvent-based carbon capture system models. This will include development of a rigorous, validated model for

the monoethanolamine (MEA) system, which will serve as a “Gold Standard” model and baseline for comparisons. MEA solvent is considered current state-of-the-art for removing CO<sub>2</sub> from existing pulverized-coal fired boilers.

- Develop and validate high-resolution submodels that more accurately predict how solvents perform under various conditions, including different packaging structures, gases, and temperatures. Apply the high-resolution submodels to simulate the performance of a solvent-based pilot-scale reactor.
- Develop and demonstrate a framework consisting of component models that are applicable to large-scale, integrated power generation systems with carbon capture, such as pre-combustion carbon dioxide (CO<sub>2</sub>) capture and oxycombustion systems, which burn a fuel using pure oxygen instead of air. The framework will be demonstrated using a set of component models for fully optimizing and analyzing a complete oxycombustion-based power plant with carbon capture, including validated models for the air separation unit, boiler, steam cycle, compression system, and CO<sub>2</sub> purification.

To learn more about the CCSI Toolset, contact [David Miller](#).

## FUNDAMENTAL FUN

### Brines in Geological Systems

**W**aters with concentrations of salts higher than that of sea water (35 g of salt per kg of sea water) are considered brines. They are found in subsurface caverns or in lakes—like the Great Salt Lake (salinity 122–280 g/kg) and the Dead Sea (salinity 300 g/kg). Some brines that NETL researchers work with have salinities 5–10 times higher than that of sea water. Brines are typically high in sodium chloride—table salt—but salts containing calcium, magnesium, or potassium can be present, too.

Brines typically result from evaporation of sea water or formation of sea ice. New brines can develop when fresher water mixes with dissolvable salt deposits like salt domes—common in the Gulf of Mexico’s sea floor—that ooze through cracks and make the surrounding water briny.

Brines can also be produced during oil and gas production as process water mixes with salts from prehistoric seas. In older producing fields, wells may yield more brine than oil. But brines don’t leave energy producers in a pickle; industry can manage those waters through treatment, reuse, or reinjection into permeable rock formations.

Brines are not just a source of table salt. Processing can make brines acceptable for industrial applications, and researchers are examining possible processes to use brines for drinking water in drier regions. Lithium—used in car batteries—and other high-value elements are found in some brines, too, and although current processing methods are pricey, future methods may make brines sought-after for these elements.

Contact: [Yee Soong](#)



NETL uses the hydrothermal-rocking autoclave test unit to study the ability of CO<sub>2</sub> to dissolve into brines.

## APPLAUSE

### Kudos!



**David Miller's** vision and leadership of the Carbon Capture Simulation Initiative (CCSI) has earned him a 2015 Arthur S. Flemming Award in Applied Science and Engineering. The Arthur S. Flemming Award was established in 1948 to honor outstanding federal employees. Recognized by the President of the

United States, agency heads, and the private sector, the winners are selected from all areas of the federal service. Miller and eleven other exceptional government employees received Flemming Awards in a ceremony on June 8, 2015.

Industry needed a more rapid and robust process to identify and scale up promising carbon capture technologies while reducing the number of costly large-scale experiments, and this need led Miller to develop CCSI. The Initiative features a multi-disciplinary team of researchers across the United States that develop new multiscale computational models and simulation tools to accelerate the development and scale up of cost-effective carbon capture technologies.

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**Joseph Licavoli, Paul Jablonski, John Sears, and Jeffrey Hawk's** poster presentation titled "High Entropy Nickel Superalloys Designed via the CALPHAD Method," won 1st prize for poster presentations at the 3rd World Conference on Integrated Computational Materials Engineering (ICME 3) held May 31-June 4, 2015 in Colorado Springs, Colorado. TMS (the Metals, Minerals, and Materials Society) sponsored this event. Joe Licavoli made the presentation.

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## EXTRA! EXTRA!

[2015 Carbon Management Technology Conference \(CMTC 2015\)](#). This conference is scheduled for November 17-19, 2015, at the Sugar Land Marriott Town Square in Sugar Land, Texas, USA. The conference will focus on carbon capture, storage, and utilization technologies that are being performed at large scale and provide options for low greenhouse gas emissions while maintaining fuel diversity for sustainable growth.



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